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Using factor score estimates in latent variable analysis

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Using factor score estimates in latent variable analysis

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GENERAL INTRODUCTION

1 Introduction

Factor analysis and structural equation modeling are commonly used in many disciplines including social, medical, business, and behavioral sciences. The use of latent factor structure is sensible in these research areas because the variables of primary interest are mainly theoretical constructs that are often observed only indirectly through a set of observable indicators. Researchers are most often interested in developing models for testing a hypothesized latent relationship and do not often consider true value estimation of the latent variable constructs. Although it is natural to use factor scores, it is not obvious how to deal with the fact that one must use estimated parameters to calculate estimates of factor scores. In addition, researchers may be interested in nonlinear relationships among the latent concepts instead of purely linear ones. Previous presentations of general methodologies for fitting nonlinear latent relationships have been limited and difficult to implement.

One particular model in which researchers are limited is nonlinear covariate factor analysis, where the interest is in assessing the efficacy of a treatment intervention. Due to a

lack of easily applied techniques, researchers tend to disregard covariate information, nonlinearity, and measurement error in assessing latent relationships.

This dissertation serves two purposes. First, we will present a statistically sound and easily applicable method of assessing intervention effects with a nonlinear relationship while incorporating covariate information, and secondly we present a way to account for measurement error in true value estimation of latent variable constructs.

2 Dissertation Organization

This dissertation consists of two papers. In the first paper, we address the problem of adjusting for covariates and incorporating nonlinear effects when attempting to assess an intervention effect. We propose an approach using estimated values of latent variables. This allows an efficient and proper assessment of the intervention effect and can also be useful in modeling potentially nonlinear relationships among latent variables. This method can be easily applied, and involves first estimating the latent variable values and then using information about covariates, and those estimated values, in a basic regression equation. Nonlinear relationships can easily be incorporated into this model. We show that this method is statistically sound and gives consistent estimates of the magnitude of the intervention effect. Simulation studies and an example from an intervention study are included.

In the second paper, we address true value estimation of latent variable constructs. Although it is natural to use factor score estimates, it is not obvious how to deal with the fact that the parameters needed for the estimation of the factor scores are themselves estimated.

Due to the lack of an explicit expression for the variance of factor score estimates, these added measurement errors have been widely disregarded. We will present a method that accounts for this extra source of variability in inference. We also develop tools for inference regarding true values and diagnostics, and include a formula for the estimate of the variance of the factor score estimate. Simulation studies and an example application from an intervention study are included.

NONLINEAR LATENT COVARIATE ANALYSIS USING FACTOR SCORE ESTIMATES

A paper to be submitted to the Journal of the American Statistical Association

Kari A. Azevedo and Yasuo Amemiya

Abstract

Latent variables have an important role in assessing the effectiveness of comparative treatment outcomes in social and behavioral studies. In such studies, the latent intervention treatment effect measured through observed indicators is often marginal or ambiguous. But most studies also contain measurements related to other latent quantities that can be used as covariates in improving the sensitivity of the intervention assessment. For example, socio-economic characteristics that pre-date the intervention are usually available. Typically, the potential covariates are also latent unobservable variables measured by a large number of observed indicators. Furthermore, the covariates' relationships to the intervention-targeted

response variable are often complex, and may require investigation/modeling. We propose an approach that estimates the values of latent variables and allows for an efficient and proper assessment of the intervention effect. This approach can also be useful in modeling potentially nonlinear relationships among latent variables.

1. Introduction

Recently, an increasing number of carefully designed intervention research projects have been proposed and conducted by social scientists. See e.g., Biglan (1995), Botvin et al. (1995), Caplan et al. (1992), Hawkins, Catalano and Miller (1992), Kellam and Rebok (1992), Perry et al. (1996), Reid (1996), Webster-Stratton and Hammond (1997), Spoth, Redmond, and Shin (1998) and West et al. (1991). Although a typical intervention study is well-designed, with proper assignments of subjects to treatment groups, the usual method for analyzing the results and for assessing the proposed programs has been linear structural equation modeling. Because most of the conceptual variables are indirectly measured, structural equation modeling using latent variables has proven to be an appropriate and useful method for exploring, describing, and modeling data in social science observational studies. However, in a well-designed intervention study, the main goal is to assess and compare different programs or treatments, and issues of modeling relationships or confirming the fit of a theoretical model are not directly relevant. This paper emphasizes the experimental, rather than the observational, aspects of social science intervention studies, and attempts to develop a useful and coherent analysis of covariance procedure.

A typical intervention study can be formulated in the following way. There are q treatments or intervention programs (including controls) to be compared for individuals (subjects, families, etc.) in a target population. Suppose that a random sample of n individuals is taken from the target population, and that the individuals are randomly assigned to the q treatments with pre-set replicate numbers n_i, $i = 1, 2, \ldots, q$ where $\sum_{i=1}^{q} n_i = n$. For the j^{th} individual in the i^{th} treatment group, let g_{ij} denote the value of a response variable used for treatment comparison. The value g_{ij} may or may not be directly observable. In some social science intervention studies, g_{ij} is called an intervention-targeted factor. As in other standard statistical comparative studies, we treat g_{ij} as independent random variables with the means possibly affected by the treatments. We write

$$g_{ij} = \mu_i + \zeta_{ij}, \quad j = 1, 2, \ldots, n_i \text{ and } i = 1, 2, \ldots, q. \tag{1.1}$$

where μ_i are unknown fixed constants, and ζ_{ij} are independent and identically distributed random variables with mean zero and variance $\sigma_{\cdot\cdot}$. If g_{ij} are observable and there are no other observable variables, then the standard F or t tests can be justified for treatment comparison whenever there is randomization, an approximate normal distribution for ζ_{ij}, and/or whenever the n_i's are large.

In social and behavioral science problems, these tests often fail to detect the treatment differences because the intervention effects, (i.e. the differences among μ_i) in (1.1) tend to be small while the individual variability as measured by $\sigma_{\cdot\cdot}$ is typically large. Also, the factor g_{ij} is usually not directly observed and must be measured indirectly by one or more

observed indicators. Then, the treatment differences need to be compared to the variability arising from both individual differences and measurement errors. Fortunately, typical social and behavioral studies also consider other latent factors that either represent concepts/states before intervention or are believed to be unaffected by the treatments. These may include pre-intervention behaviors or socio-economic characteristics. Such factors, when used as latent covariates, improve the power/sensitivity of the treatment comparison tests, provided they can reduce the variability in the individual difference term ζ_{ij}.

Some of these factors also have to be measured indirectly by observed indicators. Let f_{ij} denote a $k \times 1$ vector consisting of potential covariate factors. For the measurement structure for g_{ij} and f_{ij}, we assume the existence of separate indicator vectors y_{ij} with dimension $(p_y \times 1)$ and x_{ij} with dimension $(p_x \times 1)$, and consider the standard linear factor analytic models in the errors-in-variables parameterization

$$y_{ij} = \begin{pmatrix} \alpha_0 \\ 0 \end{pmatrix} + \begin{pmatrix} \alpha_1 \\ 1 \end{pmatrix} g_{ij} + \varepsilon_{yij}, \tag{1.2}$$

$$x_{ij} = \begin{pmatrix} \beta_0 \\ 0 \end{pmatrix} + \begin{pmatrix} \beta_1 \\ I_k \end{pmatrix} f_{ij} + \varepsilon_{xij}, \tag{1.3}$$

where unknown parameters $\alpha_0, \alpha_1, \beta_0$ and β_1 may contain further restrictions such as zero elements, and ε_{yij} and ε_{xij} are random vectors with mean zero. It is assumed that, for all $j = 1, 2, \ldots, n_i$ and $i = 1, 2, \ldots, q$ that ζ_{ij}, ε_{yij} and ε_{xij} are mutually independent, and that $(\zeta_{ij}, \varepsilon'_{yij}, \varepsilon'_{xij})$ are identically distributed with mean zero. We do not necessarily assume that any of the three error terms are normally distributed. We also leave the distributional form

for the latent covariate f_{ij} as unspecified, including the case of correlated (e.g., longitudinally) or fixed f_{ij}. Since the error term ζ_{ij} and the factor f_{ij} both represent individual characteristics/differences, some association between them is expected to be present. However, we do not specify any particular form of relationship for such association at this point, and in (1.3), if an element of f_{ij} is observed without error, then one element of x_{ij} is identically equal to that element of f_{ij}. In (1.2), if only one observed indicator is available for g_{ij}, then we write $y_{ij} = g_{ij}$, and the equation error ζ_{ij} is assumed to contain the confounded measurement error. With this understanding, each of the measurement models (1.2) and (1.3) is assumed to be identified, i.e., all unknown elements in α_0, α_1, $\Upsilon = Var\{\varepsilon_{yij}\}$, β_0, β_1 and $\Psi = Var\{\varepsilon_{xij}\}$ can be estimated.

The basic intuitive approach for covariate analysis in this setting is to combine the information in y_{ij} to obtain some estimate of g_{ij}, and to use functions of x_{ij} as covariates. The most appropriate and effective covariates would be the elements of f_{ij} and their functions representing the individual characteristics unrelated to the treatments, if they were observable. On the other hand, observed indicators in x_{ij} are contaminated with measurement errors, and their association with the individual variability ζ_{ij} is only through f_{ij}. Latent covariate analysis addresses how to use the observed x_{ij} to carry out analysis of covariance in an effective, appropriate and flexible way.

Because the individual factor f_{ij} represents an interpretable and meaningful concept, the subject-matter theory often suggests a general form or tendency of the relationship

between the response g_{ij} and f_{ij} (in terms of f_{ij}, not x_{ij}). For example, in social intervention program studies, some pre-intervention measures of risk behaviors are often obtained. With or without effective intervention, the association between the risk factor and the response or resulting outcome is usually considered nonlinear, because subjects with moderate to large risk may change their behavior over time while those with low risk at the start tend to stay unchanged or have little room for improvement. Hence, in many social and behavioral studies, methods for incorporation of nonlinear covariate adjustments may be particularly useful in assessing and comparing intervention programs. Extensions of our approach to different study designs e.g., involving blocking, repeated measures, and/or within-subgroup comparisons are relatively straightforward. Our discussion here concentrates on the rather simple setting of (1.1), (1.2), and (1.3), so that the important issues and our original approach can be understood easily.

In the current practice of social and behavioral intervention studies, two methods are commonly used for incorporating covariates in improving the treatment comparison. In the context of model (1.1) - (1.3), one method, applicable only with $p_v = 1$, is the usual regression analysis for y_{ij} including all observed indicators in x_{ij} linearly. This approach does not use the latent variable structure in (1.3), and uses large numbers of covariates rather inefficiently simply for the purpose of incorporating covariate effects. Another method assumes the existence of a linear structural model between g_{ij} and f_{ij}, and fits the overall structural equation model treating every random variable involved as normal. One difficulty with a structural model based approach is the heavy reliance on the linear model and normality assumptions. The covariate f_{ij} may not be utilized in the most efficient way, and

the treatment comparison inference may be affected by some detailed violation of the assumed model. Neither of these two methods can accommodate any covariate effects other than simple linear relationships. In the regression with the observed indicators, the number of covariates can become very large, e.g., if all quadratic functions of the elements of x_{ij} are included. In the structural equation approach, the use of nonlinear structural models has not been developed fully, especially with possibly nonnormal f_{ij}.

A standard reference for latent covariate analysis is Aiken, Stein, and Bentler (1994) who used the covariate structure analysis method for a simple situation. They considered a linear relation between covariates and outcome, using one post intervention measurement and no group experimental-unit effect. They described two structural equations methods that can be used in the evaluation of intervention-control group differences on multiple outcomes. One of these is a multi-group structured means analysis that splits the sample into intervention and control groups, estimates a separate measurement model for each group, and tests the differences between construct means in those groups. The alternative uses a common measurement model for both groups and includes a group code dummy variable and has paths in the structural model from the group code variable to relevant outcome constructs. The major advantage of the group code approach is that it requires estimating fewer parameters, reducing the required sample size. In the discussion portion of their paper, Aiken et al. propose that the strategy of using categorically coded treatment variables in the analysis of group differences will lead to more successful modeling than structural mean analysis.

The main shortcomings of the Aiken et al. proposed analysis are that they are limited exclusively to the use of linear covariates and the results of the analysis are dependent on the construction of the measurement model. Also, the analysis relies on the normality of the covariates. Russell et al. (1998) also advocate the use of the structural equations modeling approach. Carroll et al. (1985) explore the conjecture that, when the least squares estimate is consistent for a linear combination of the regression parameters, it will be preferred to an errors-in-variables estimate, at least asymptotically. They show this to be true for randomized two-group analysis of covariance. This suggests that possible higher efficiency of using the observation regression approach may be more efficient than traditional ML modeling. This is the direction in which we expand to the use of nonlinear covariates.

Considerable methodological development has been achieved in linear latent variable analysis, but at the present time there are few reliable and practical methods for incorporating nonlinear covariates to further reduce variability. The methods that are available tend to be inconvenient and difficult to implement. These include using the actual covariate values or functions of them. However, the difficulties associated with using all elements of x_{ij} and their functions as covariates increase as the number of regressor variables increases. We will present a more efficient and suitable way to incorporate these nonlinear covariates.

Others have presented methods for nonlinear latent variable analysis. The much cited Kenny and Judd (1984) paper established a method of using product indicators for fitting latent interaction terms and latent quadratic terms. Wall and Amemiya (2001) proved that the Kenny-Judd procedure produces an inconsistent parameter estimator for most practical situations. Wall and Amemiya's generalized appended product indicators (GAPI) procedure

has no such limitations. However, none of these are focused on the main point of interest, which is the detection of intervention effects.

Existing nonlinear procedures are limited in that they can only incorporate latent quadratic or interaction terms. A general nonlinear form is not as simple, and with the latent covariate method, we aren't limited to strictly quadratic or interaction effects to assess for an intervention effect. We will show that we get correct results adjusting for covariates and incorporating a nonlinear effect. We will also show that in latent covariate analysis, where the emphasis is on correct inference for the magnitude of the intervention effect, these methods perform better than other currently available methods.

2. Latent Covariate Method

We first assume that there is more than one observed indicator for the response factor g_{ij} in (1.2). Then, for each of the two measurement models (1.2) and (1.3), we apply a model-fitting procedure (treating g_{ij} unrestricted) that is known to produce consistent parameter estimators without specifying the distributions of the factors and errors. For example, the maximum likelihood estimator under assumed normality can be used. An additional advantage of using normal maximum likelihood estimation is that asymptotic inferences for the model parameters can be carried out easily. See, e.g., Anderson and Amemiya (1988), Browne and Shapiro (1988) and Amemiya and Anderson (1990). We denote such parameter estimators by $\hat{\alpha}_0$, $\hat{\alpha}_1$, $\hat{\Upsilon}$, $\hat{\beta}_0$, $\hat{\beta}_1$ and $\hat{\Psi}$.

The next step in our approach is to obtain the factor score estimators for g_{ij} and f_{ij} treating them as fixed constants, i.e., using Bartlett's method. The straightforward forms of the score estimators for nonsingular Ψ and Υ are

$$\hat{f}_{ij} = \left[\left(\hat{\beta}_1', I_k \right) \hat{\Psi}^{-1} \begin{pmatrix} \hat{\beta}_1 \\ I_k \end{pmatrix} \right]^{-1} \left(\hat{\beta}_1', I_k \right) \hat{\Psi}^{-1} \left[x_{ij} - \begin{pmatrix} \hat{\beta}_0 \\ 0 \end{pmatrix} \right]$$

$$\hat{g}_{ij} = \left[\left(\hat{\alpha}_1', 1 \right) \hat{\Upsilon}^{-1} \begin{pmatrix} \hat{\alpha}_1 \\ 1 \end{pmatrix} \right]^{-1} \left(\hat{\alpha}_1', 1 \right) \hat{\Upsilon}^{-1} \left[y_{ij} - \begin{pmatrix} \hat{\alpha}_0 \\ 0 \end{pmatrix} \right].$$

The forms more appropriate for the cases with some observable factors or singular error covariance matrix estimates amount to applying a one-to-one transformation to the $p_x \times 1$ observation x_{ij} to obtain

$$\hat{f}_{ij} = \left[-\hat{\Gamma}_x, \left(I_k + \hat{\Gamma}_x \hat{\beta}_1 \right) \right] \left[x_{ij} - \begin{pmatrix} \hat{\beta}_0 \\ 0 \end{pmatrix} \right] \tag{2.1}$$

where

$$\hat{\Gamma}_x = \left(0, I_k \right) \hat{\Psi} \begin{pmatrix} I_{(p_x - k)} \\ -\hat{\beta}_1' \end{pmatrix} \left[\left(I_{(p_x - k)}, -\hat{\beta}_1 \right) \hat{\Psi} \begin{pmatrix} I_{(p_x - k)} \\ -\hat{\beta}_1' \end{pmatrix} \right]^{-1}. \tag{2.2}$$

Similarly, we can apply a one-to-one transformation to the $p_y \times 1$ observation y_{ij} to obtain

$$\hat{g}_{ij} = \left[-\Gamma_y, \left(1 + \hat{\Gamma}_y \hat{\alpha}_1 \right) \right] \left[y_{ij} - \begin{pmatrix} \hat{\alpha}_0 \\ 0 \end{pmatrix} \right] \tag{2.3}$$

where

$$\hat{\Gamma}_y = \left(0, 1 \right) \hat{\Upsilon} \begin{pmatrix} I_{(p_y - k)} \\ -\hat{\alpha}_1' \end{pmatrix} \left[\left(I_{(p_y - k)}, -\hat{\alpha}_1 \right) \hat{\Upsilon} \begin{pmatrix} I_{(p_y - k)} \\ -\hat{\alpha}_1' \end{pmatrix} \right]^{-1}. \tag{2.4}$$

Under (1.1), we can write

$$\hat{g}_{ij} = \mu_i + \zeta_{ij} + \xi_{ij} = \mu_i + \eta_{ij}, \tag{2.5}$$

where $\xi_{ij} = \hat{g}_{ij} - g_{ij}$ is the estimation error independent of ζ_{ij} and ε_{xij} in (1.3). If only one indicator y_{ij} for g_{ij} is available, we set $\hat{g}_{ij} = y_{ij}$, and the measurement error in y_{ij} and the individual differences ζ_{ij} are confounded. The method for latent covariate analysis is to perform tests comparing μ_i in model (2.5) using functions of the elements of $\hat{f}_{ij}$ as covariates and treating η_{ij} as an independent and identically distributed error term with unknown variance.

The covariate $\hat{f}_{ij}$ is expected to reduce the part of error variability due to the individual differences ζ_{ij}, but not the measurement error part ξ_{ij}, and $\hat{f}_{ij}$ is not as effective of a covariate as f_{ij} would be. However, compared to using the elements of x_{ij} and their functions without using measurement model structure, $\hat{f}_{ij}$ serves as a way to combine the relevant information in a manner consistent with the overall setting without increasing the number of covariates unnecessarily. Also, the use of $\hat{f}_{ij}$ allows a simple data analytic way to identify the form of covariate relationships. For this, we suggest examining scatter plots of $\hat{g}_{ij} - \bar{\hat{g}}_{i\cdot}$ versus the elements of $\hat{f}_{ij} - \bar{\hat{f}}_{i\cdot}$, and their simple functions, where $\bar{\hat{g}}_{i\cdot} = \frac{1}{n_i}\sum_{j=1}^{n_i} \hat{g}_{ij}$ and $\bar{\hat{f}}_{i\cdot} = \frac{1}{n_i}\sum_{j=1}^{n_i} \hat{f}_{ij}$. This graphical method should be informative and sufficient for deciding what functional form of the covariate relationship and what functions of the elements can be tried out in analysis. Also, some theoretical consideration of the meaning of the true f_{ij} may lead to a preference for a particular functional form over others. For example, with an element of

f_{ij} representing risk behavior or basic social skills, we might suspect some nonlinear covariate relation, in which case an approximate quadratic function may be more effective as a covariate than a linear one. We also note that, with primary interest in comparing the treatments effectively, searching for a precise covariate relation or examining a particular functional form rigorously is largely irrelevant.

Let $h(f_{ij};\gamma)$ denote the parametric function suggested, based on the scatter plots or theoretical consideration, as a possible relationship between the response g_{ij} and f_{ij} except for the treatment differences. Here, the parameter vector γ is unknown. For example, for a quadratic covariate adjustment using a scalar f_{ij}, we would suggest using the function $h(f_{ij};\gamma) = \gamma_0 + \gamma_1 f_{ij} + \gamma_2 f_{ij}^2$. Then, latent covariate analysis applies the standard nonlinear regression to fit $\mu_i + h(\hat{f}_{ij},\gamma)$ to $\hat{g}_{ij}$ by least squares, i.e., minimize

$$\sum_{i=1}^{q}\sum_{j=1}^{n_i}\left[\hat{g}_{ij} - \mu_i + h(\hat{f}_{ij};\gamma)\right]^2 \qquad (2.6)$$

with repect to μ_i, $i = 1,2,\ldots,q$ and γ. We propose using the resulting estimators of μ_i and their asymptotic covariances/standard errors to perform the treatment comparison tests. For possible finite-sample accuracy, we suggest the use of t-tests and F-tests with (denominator) degrees of freedom $d = n - q - \dim(\gamma)$.

Mathematical justification for the appropriateness of this analysis using $\hat{f}_{ij}$ from (2.1) in any nonlinear covariate adjustments is given in the next section.

3. Asymptotic Theory

In this section, theoretical justification is given for the latent covariate analysis method proposed in Section 2. Throughout, we assume

(a) Models (1.1), (1.2) and (1.3) hold.

(b) Three error terms ζ_{ij}, ε_{yij} and ε_{xij} are independent, and $\left(\zeta_{ij}, \varepsilon'_{yij}, \varepsilon'_{xij}\right)'$ $j = 1, 2, \ldots, n_i$, $i = 1, 2, \ldots, q$ are independent, identically distributed with mean zero and finite fourth moments.

(c) The factors f_{ij}, $j = 1, 2, \ldots, n_i$, $i = 1, 2, \ldots, q$ are independent of all ε_{yij} and ε_{xij}, and are independent, identically distributed with finite second moments.

(d) As $n \to \infty$, $\frac{n_i}{n} \to c_i$, $i = 1, 2, \ldots, q$, where $0 < c_i < \infty$ and $\sum_{i=1}^{q} c_i = 1$

Note that assumption (c) includes the conditions necessary for the unobservable f_{ij} to be considered an appropriate covariate, namely, the distribution of f_{ij} is identical for all treatment groups $i = 1, 2, \ldots, q$. This condition holds if a random sample of n individuals is taken from the target population with the individual characteristics represented by f_{ij}, and if the n individuals are randomly divided into the q treatment groups of pre-set sizes n_i, $i = 1, 2, \ldots, q$. Assumption (c) can be replaced by some limiting conditions without restricting to independent identically distributed f_{ij}. But, for simplicity, we use (c) here so the basic issues can be understood easily. Let $\hat{\theta}$ denote a vector consisting of the elements in $\hat{\alpha}_0$, $\hat{\alpha}_1$, $\hat{\Upsilon}$, $\hat{\beta}_0$, $\hat{\beta}_1$ and $\hat{\Psi}$, and let θ be the true parameter value. Assumptions (a)-(d) are sufficient

for the maximum likelihood estimator under normality to be consistent for θ. Since we allow the use of other types of $\hat{\theta}$, we assume

(e) As $n \to \infty$, $\hat{\theta} \to \theta$, a.s., and $\hat{\theta} - \theta = O_p\left(n^{-1/2}\right)$.

Using the elements of the true θ, define

$$\ddot{g}_{ij} = g_{ij} + s_{ij}, \tag{3.1}$$

$$\ddot{f}_{ij} = f_{ij} + r_{ij},$$

where $s_{ij} = \left[(0,1) - \Gamma_y\left(I_{p_1-k}, -\alpha_1\right)\right]\varepsilon_{yij}$ and $r_{ij} = \left[(0, I_k) - \Gamma_x\left(I_{p_1-k}, -\beta_1\right)\right]\varepsilon_{xij}$ with Γ_y and Γ_x as defined in (2.4) and (2.2).

We need the following lemma concerning the factor score estimators $\hat{g}_{ij}$ in (2.3) and $\hat{f}_{ij}$ in (2.1).

Lemma 1. We can write

$$\hat{g}_{ij} = \ddot{g}_{ij} + b_{ij}'\left(\hat{\theta} - \theta\right),$$

$$\hat{f}_{ij} = \ddot{f}_{ij} + B_{ij}\left(\hat{\theta} - \theta\right),$$

where any element b_{ij} of either b_{ij} or B_{ij} is a linear function of either $\left(g_{ij}, \varepsilon_{yij}'\right)$ or $\left(f_{ij}', \varepsilon_{xij}'\right)$ with coefficients depending on $\hat{\theta}$.

Proof. The expressions were derived in Wall and Amemiya (2000). □

In the latent covariate model, ζ_{ij} and f_{ij} characterize individuals, and so they are expected to be dependent of each other. In latent covariate analysis, we choose the function $h(\cdot;\gamma)$ with an aim that the variance of $\zeta_{ij} - h\left(f_{ij};\gamma\right)$ with the best choice of γ is

substantially smaller than $\sigma_{\zeta\zeta}$. We need to assume some condition on the function $h(\cdot;\gamma)$. But, the conditions are expressed in terms of $\ddot{f}_{ij}$, since $\hat{f}_{ij}$ is used in place of the unobservable f_{ij}. Let Ω denote the parameter space for γ. We assume

(f) The function $h(f;\gamma)$ is continuous in γ for every f. Also, the distributions of ζ_{ij}, f_{ij} and $\varepsilon_{xij}\varepsilon_{yij}$ are such that, for each i, as $n \to \infty$,

$$\frac{1}{n_i}\sum_{j=1}^{n_i}\left[h\left(\ddot{f}_{ij};\gamma\right), h^2\left(\ddot{f}_{ij};\gamma\right), \zeta_{ij}h\left(\ddot{f}_{ij};\gamma\right), s_{ij}h\left(\ddot{f}_{ij};\gamma\right)\right] \to \left[H_1(\gamma), H_2(\gamma), H_3(\gamma), 0\right]$$

a.s., uniformly for all γ in Ω.

(g) Let $D^{(w)}(f;\gamma)$ denote a matrix of all w^{th} order partial derivatives of $h(f;\gamma)$ with respect to f. Then for some positive integer w_0, there exists a function $H(\gamma)$ such that $D^{(w_0)}(f;\gamma)$ exists, and

$$\left|D^{(w_0)}\left(f^{(1)};\gamma\right) - D^{(w_0)}\left(f^{(2)};\gamma\right)\right| \le H(\gamma)\left|f^{(1)} - f^{(2)}\right|.$$

For the same w_0, the $2(w_0+1)^{st}$ moments of f_{ij} and ε_{xij} exist, and for each $w < w_0$,

$$\frac{1}{n_i}\sum_{j=1}^{n_i}\left|D^{(w)}\left(\ddot{f}_{ij};\gamma\right)\right|^2$$

converges almost surely to a non-random function of γ uniformly in γ.

(h) A function of γ

$$\begin{aligned} Var\left\{\zeta_{ij} - h\left(\ddot{f}_{ij};\gamma\right)\right\} &= \sigma_{\zeta\zeta} - 2Cov\left\{\zeta_{ij}, h\left(\ddot{f}_{ij};\gamma\right)\right\} + Var\left\{h\left(\ddot{f}_{ij};\gamma\right)\right\} \\ &= \sigma_{\zeta\zeta} - 2H_3(\gamma) + H_2(\gamma) - H_1^2(\gamma) \end{aligned}$$

is uniquely minimized over Ω at $\gamma = \gamma^0$, where $H_1(\gamma)$, $H_2(\gamma)$ and $H_3(\gamma)$ are given in (f).

Note that the limits in (f) are free of i under (b) and (c). The assumption (g) holds automatically for any $h(f;\gamma)$ polynomial in f of order r, provided that the $(2r)^{th}$ moments of f_{ij} and ε_{xij} exist. The value γ^0 in (h) is the "true" value being estimated by $\hat{\gamma}$, although the estimation of the γ parameter is irrelevant in analysis of covariance. The function $h(\cdot;\gamma)$ is usually a suggested relationship based on the interpretation of the true factor score f_{ij}. But, the use of $\hat{f}_{ij}$ in place of f_{ij} results in utilizing $h(\hat{f}_{ij};\gamma^0)$ as the covariate.

Recall that the latent covariate method obtains relevant statistics by minimizing (2.6). Clearly, for any given value of γ, (2.6) is minimized by setting

$$\hat{\mu}_i(\gamma) = \bar{\hat{g}}_{i\cdot} - \frac{1}{n_i}\sum_{j=1}^{n_i} h(\hat{f}_{ij};\gamma), \tag{3.2}$$

where

$$\bar{\hat{g}}_{i\cdot} = \frac{1}{n_i}\sum_{j=1}^{n_i} \hat{g}_{ij}.$$

By substituting this into (2.6), we see that the estimator $\hat{\gamma}$ is the value minimizing

$$P(\gamma) = \frac{1}{n}\sum_{i=1}^{q}\sum_{j=1}^{n_i}\left\{\hat{g}_{ij} - \bar{\hat{g}}_{i\cdot} - \left[h(\hat{f}_{ij};\gamma) - \frac{1}{n_i}\sum_{j=1}^{n_i} h(\hat{f}_{ij};\gamma)\right]\right\}^2$$

over Ω.

The next lemma shows that $\hat{\gamma}$ is consistent for γ^0 in (h).

Lemma 2. Assume (a)-(h). Then as $n \to \infty$,

$$\hat{\gamma} \to \gamma^0 \text{, a.s..}$$

Proof. We first obtain the exact Taylor expansion of $P(\gamma)$ with respect to $\hat{f}_{ij}$ around $\ddot{f}_{ij}$ up to the w_0^{th} power term, where w_0 is as specified in (g). By substituting this expansion into $P(\gamma)$, and by carefully examining each term in the sum of squares utilizing (g) and Lemma 1, we obtain that

$$P(\gamma) - \ddot{P}(\gamma) \to 0 \text{, a.s.,}$$

uniformly for all γ in Ω, where

$$\ddot{P}(\gamma) = \frac{1}{n}\sum_{i=1}^{q}\sum_{j=1}^{n_i}\left\{\ddot{g}_{ij} - \bar{\ddot{g}}_{i\cdot} - \left[h\left(\ddot{f}_{ij};\gamma\right) - \frac{1}{n_i}\sum_{j=1}^{n_i} h\left(\ddot{f}_{ij};\gamma\right)\right]\right\}^2,$$

$$\bar{\ddot{g}}_{i\cdot} = \frac{1}{n_i}\sum_{j=1}^{n_i}\ddot{g}_{ij}.$$

Substituting (1.1) and (3.1), we can write

$$\ddot{P}(\gamma) = \frac{1}{n}\sum_{i=1}^{q}\sum_{j=1}^{n_i}\left[s_{ij} + \zeta_{ij} - h\left(\ddot{f}_{ij};\gamma\right)\right]^2 - \sum_{i=1}^{q}\frac{n_i}{n}\left[\bar{s}_{i\cdot} + \bar{\zeta}_{i\cdot} - \frac{1}{n_i}\sum_{j=1}^{n_i} h\left(\ddot{f}_{ij};\gamma\right)\right]^2,$$

where

$$\left(\bar{s}_{i\cdot}, \bar{\zeta}_{i\cdot}\right) = \frac{1}{n_i}\sum_{j=1}^{n_i}\left(s_{ij}, \zeta_{ij}\right) = O_p\left(n^{-1/2}\right).$$

Thus, by (f),

$$P(\gamma) \to \sigma_{ss} + \sigma_{\zeta\zeta} - 2H_3(\gamma) + H_2(\gamma) - H_1^2(\gamma) \text{, a.s.,} \qquad (3.3)$$

where $H_1(\gamma)$, $H_2(\gamma)$ and $H_3(\gamma)$ are defined in (f), $\sigma_{ss} = Var\{s_{ij}\}$ for the measurement error s_{ij} in (3.1), and $\sigma_{\zeta\zeta} = Var\{\zeta_{ij}\}$ is the individual variability in (1.1). Now, the strong consistency of $\hat{\gamma}$ for γ^0 follows from (3.3), (h) and the standard argument. □

The following theorem shows the consistency of the covariate analysis estimator of any contrast among the treatment means μ_i, $i = 1, 2, \ldots, q$.

Theorem 1. Let $\tau = \sum_{i=1}^{q} a_i \mu_i$ denote the contrast with $\sum_{i=1}^{q} a_i = 1$, and let τ^0 denote the true value. Let $\hat{\tau} = \sum_{i=1}^{q} a_i \hat{\mu}_i(\hat{\gamma})$ be the analysis of covariance estimator of τ obtained by minimizing (2.6), i.e., using (3.2). Under (a)-(h), as $n \to \infty$,

$$\hat{\tau} \to \tau^0, \text{ a.s..}$$

Proof. Assumptions (f) and (g) combined with Lemma 2 imply that

$$\frac{1}{n_i} \sum_{j=1}^{n_i} h(\hat{f}_{ij}; \hat{\gamma}) \to H_1(\gamma^0), \text{ a.s.,}$$

which is free of i. Hence, the result follows from (3.2). □

Thus, although $\hat{\mu}_i$ is not consistent for μ_i (but for $\mu_i - H_1(\gamma^0)$), any contrast among μ_i's can be consistently estimated by the same linear combination of $\hat{\mu}_i$'s. To obtain the asymptotic distribution of the contrast estimator $\hat{\tau}$, we assume

(i) The true value of γ^0 is an interior point of Ω. Let $F^{(\upsilon_0)}(f;\gamma)$ denote the matrix for some integer $\upsilon_0 \geq 2$ of all υ_0^{th} order partial derivatives of $h(f;\gamma)$ with respect to γ. Then

$$\frac{1}{n_i}\sum_{j=1}^{n_i}\left|F^{(u_0)}\left(\ddot{f}_{ij};\gamma\right)\right|^2$$

converges almost surely as $n\to\infty$ uniformly in γ.

The next theorem shows that the covariate analysis contrast estimator $\hat{\tau}$ is unaffected in large samples by the estimation error in $\hat{\theta}$, i.e., the use of $\hat{f}_{ij}$ in place of $\ddot{f}_{ij}$.

Theorem 2. Assume (a)-(i). The analysis of covariance estimator $\hat{\tau}$ of τ^0 in Theorem 1 satisfies, as $n\to\infty$,

$$\hat{\tau}-\tau^0=\sum_{i=1}^{q}a_i u_i+o_p\left(n^{-1/2}\right),$$

where

$$u_i=\bar{s}_{i\cdot}+\bar{\delta}_{i\cdot}=\frac{1}{n_i}\sum_{j=1}^{n_i}\left(s_{ij}+\delta_{ij}\right),$$

$$\delta_{ij}=\zeta_{ij}-\left[h\left(\ddot{f}_{ij};\gamma^0\right)-H_i\left(\gamma^0\right)\right].$$

Proof. Using Lemma 1 and assumptions (e)-(g), we can show that

$$\frac{1}{n_i}\sum_{j=1}^{n_i}h\left(\hat{f}_{ij};\hat{\gamma}\right)=\frac{1}{n_i}\sum_{j=1}^{n_i}h\left(\ddot{f}_{ij};\hat{\gamma}\right)+R'(\hat{\gamma})\left(\hat{\theta}-\theta\right)+o_p\left(n^{-1/2}\right) \tag{3.4}$$

where $R(\gamma)$ is a non-random continuous function of γ free of i. Also, using assumptions (f), (g) and (i) as well as Lemma 2 in expanding the derivative of $P(\gamma)$ with respect to γ evaluated at $\hat{\gamma}$, we can show that $\hat{\gamma}-\gamma^0=O_p\left(n^{-1/2}\right)$. Applying this order result and (i) in (3.4), we obtain

$$\frac{1}{n_i}\sum_{j=1}^{n_i}h\left(\hat{f}_{ij};\hat{\gamma}\right)=\frac{1}{n_i}\sum_{j=1}^{n_i}h\left(\ddot{f}_{ij};\gamma^0\right)+R_0'\left(\hat{\theta}-\theta\right)+F_0'\left(\hat{\gamma}-\gamma^0\right)+o_p\left(n^{-1/2}\right), \tag{3.5}$$

where $R_0 = R(\gamma^0)$ and F_0 are constants free of i. Thus, combining (1.1), (3.1), (3.2) and (3.5), we have

$$\hat{\mu}_i - \mu_i = \bar{s}_{i\cdot} + \bar{\delta}_{i\cdot} - (b_0 + R_0)'(\hat{\theta} - \theta) - F_0(\hat{\gamma} - \gamma^0) + o_p(n^{-1/2}),$$

where b_0 is the constant probability limit of $\frac{1}{n_i}\sum_{j=1}^{n_i} b_{ij}$ for b_{ij} given in Lemma 1. Hence, the result follows, noting that $\sum_{i=1}^{q} a_i = 0$ and that $H_1(\gamma^0)$ is free of i. □

The next theorem gives two possible estimators of the asymptotic variance of the contrast estimator $\hat{\tau}$.

Theorem 3. Assume (a)-(i). Then, as $n \to \infty$,

$$\sqrt{n}(\hat{\tau} - \tau^0) \to^d N(0, \sigma_{\tau\tau}),$$

where

$$\sigma_{\tau\tau} = \sigma^2 \sum_{i=1}^{q} \frac{a_i^2}{c_i},$$

$$\sigma^2 = Var\{s_{ij}\} + Var\{\zeta_{ij} - h(\ddot{f}_{ij}; \gamma^0)\}.$$

Let $\hat{\sigma}^2$ denote the residual mean squares obtained by minimizing (2.6), and let $\hat{V}_1$ be the usual nonlinear regression asymptotic variance estimator for $\hat{\tau}$. Also, let

$$\hat{V}_2 = \hat{\sigma}^2 \sum_{i=1}^{q} \frac{a_i^2}{n_i}.$$

Then, as $n \to \infty$,

$$n\hat{V}_\ell \to^p \sigma_{\tau\tau}, \qquad \ell = 1, 2.$$

Proof. The limiting distribution result follows from Theorem 2 and the standard central limit theorem. The argument used in the proofs of Theorems 1 and 2 can be used to show the consistency of $\hat{\sigma}^2$ for σ^2, and the variance estimator results follow. □

Although Theorem 3 is given, for simplicity, in terms of a single contrast, the result can be extended to any number of contrasts. This theorem and its extension directly justify the use of asymptotic tests and confidence statements based on normal or chi-squared distributions. In practice, for better small sample approximation and for matching special cases with exact results, we recommend the use of t and F procedures with the error degrees of freedom $n-q-\dim(\gamma)$.

4. Simulation Studies

Simulation studies were conducted to highlight some of the differences in statistical methods when dealing with nonlinear latent covariate analysis. The factor score estimate methods, labeled Nonlinear Latent Covariate Method (NLCM), are compared to a linear version of the factor score estimate methods (LLCM) and also to linear structural equations modeling (LSEM). They are also compared with Wall and Amemiya's (2001) generalized appended product indicator procedure (GAPI) which uses products of observed variables as indicators for nonlinear terms in the structural model while constructing the model covariance matrix with no assumption on the distributional form of any of the variables in the model. We also include Bollen's (1989) instrumental variable method which uses a limited information estimator based on a two-stage least squares procedure utilizing instrumental

variables chosen such that they are correlated with an endogenous explanatory variable, but uncorrelated with the disturbance term. Usual regression analysis for y_{ij} including all of the observed indicators x_{ij} linearly and then also linearly plus quadratically were simulated. We compared the outcomes of these methods based on bias, confidence interval coverage, power, and mean square error for the estimation of the intervention effect. Lastly, we also compare the results with a simple analysis of a comparison of means of the outcomes that ignores entirely the available covariate information.

The following model was used for the indicator variables,

$$\begin{pmatrix} x_{1ij} \\ x_{2ij} \\ x_{3ij} \\ x_{4ij} \end{pmatrix} = \begin{pmatrix} 0 \\ .15 \\ .1 \\ .05 \end{pmatrix} + \begin{pmatrix} 1 \\ 0.9 \\ 1.1 \\ 1.2 \end{pmatrix} f_{ij} + \varepsilon_{xij}, \qquad \text{i = 1,2 and j = 1,..., } n_i .$$

From the model (1.1), we have that

$$y_{ij} = \mu_i + \zeta_{ij}, \quad \text{i = 1,2 and j = 1,..., } n_i,$$

where we are using a single observed indicator y_{ij} for g_{ij} and it should be noted that the equation error ζ_{ij} is assumed to contain the confounded measurement error. We used a basic quadratic model

$$h(f_{ij};\gamma) = \gamma_0 + \gamma_1 D_i + \gamma_2 f_{ij} + \gamma_3 f_{ij}^2 \qquad (4.1)$$

where D_i is the dichotomized treatment group indicator.

For each set of simulations, there are 3 different distributions used for f_{ij} : Normal (5,1), Chi-Square with 6 df, standardized and shifted to (5,1), and Gamma (4,4), also standardized and shifted to (5,1). The error variance of the structural model is

$\text{var}(\varepsilon_{yij}) = (0.2 \cdot \text{var}(-4(f_{ij} - 7)^2)$, and for the measurement model, each $\text{var}(\varepsilon_{ij}) = 0.2$. The simulations used sample sizes of 100 and 300. For the quadratic cases, we used in (4.1), $\{\gamma_0 = -16, \gamma_1 = 0.0, 1.0, 2.0, \gamma_2 = 56, \gamma_3 = -4\}$, and for the linear cases, we used in (4.1), $\{\gamma_0 = 12, \gamma_1 = 1.0, 2.0, \gamma_2 = 24, \gamma_3 = 0\}$. The model is estimated 1000 times for each simulation. Results of the simulations are provided for a mixed subset of quadratic and linear distributions, sample sizes, and true values of the intervention parameter, γ_1, for the structural model in (4.1) are presented in Tables 4.1 through 4.11.

The information given in each of the tables is the bias of the 1000 estimates of the parameter and the average of the standard error estimates. Also, the coverage of 95% confidence intervals, given as the percent of confidence intervals constructed from the estimates of the parameters and their standard errors that contain the true value of γ_1, using z=1.96. Then the power is given as the number of statistics such that the absolute value of the estimate divided by the standard error of the estimate > 1.96. Lastly, we report the mean square errors for each method.

The labels used in the tables for each of the methods are as follows. The nonlinear latent covariate method, NLCM1, is regression of (4.1). A second application of the latent covariate method, NLCM2, is regression of y_{ij} on 1, $\hat{f}_{ij}$ and $\hat{f}_{ij}^2$. Then save the residuals, R_{ij}, and regress R_{ij} on $(D_i - \bar{D})$. LLCM1 is the regression of y_{ij} on 1, D_i and $\hat{f}_{ij}$, (NLCM1 without the quadratic squared term.) LLCM2 is the regression of the residual, R_{ij}, (from y_{ij} on 1 and $\hat{f}_{ij}$) on $D_i - \bar{D}$, (NLCM2 without the quadratic squared term.) LSEM1 is the outcome from linear structural equations analysis using Proc CALIS in SAS with

$\text{cov}(D_i, f_{ij})$ estimated. LSEM2 is the same as LSEM1 except without $\text{cov}(D_i, f_{ij})$ estimated. GAPI is Wall and Amemiya's (2001) generalized appended product indicator procedure with $x_{1j} * x_{2j}$ as the product indicator using Proc CALIS in SAS. Bollen is Bollen's (1989) instrumental variable method with y_{ij}, x_{1j}, and x_{1j}^2 as the endogenous variables, x_{2j}, x_{3j}, x_{4j} and $x_{1j} * x_{2j}$ as instruments with the model y_{ij} on D_i, x_{1j}, x_{1j}^2 using Proc SYSLIN in SAS with the 2SLS option. REG1 is regression of y_{ij} on the observed x_{ij} variables. REG2 is the regression of y_{ij} on the observed variables, the x_{ij}'s, and the squares of the x_{ij}'s. The final row of the tables includes NoCov, which is the analysis of the difference in treatment effect estimates when ignoring all available covariate information.

It is evident that in the estimation of the treatment effect, γ_1 from (4.1), the latent covariate methods are repeatedly shown to create less bias, lower standard errors, better confidence interval coverage, higher power, and lower mean square error than the other methods. We note that in many of the simulations, the simple REG2 seems to perform fairly well. However, in practical situations, when the x_{ij} vector contains increasingly more than 4 variables, the bias increases substantially where as NLCM1 and NLCM2 do not. Also, it is clear that ignoring relevant covariate information in the analysis achieves very little in the way of inference.

Table 4.1 with Quadratic, Normal, $n_1 = 50$, $n_2 = 50$, $\gamma_1 = 0$

Method	Bias	Ave. Std. Err.	CI coverage	Power	MSE
NLCM1	-0.122	2.13	94.6	54	4.57
NLCM2	-0.123	2.10	94.5	55	4.41
LLCM1	-1.546	2.08	94.1	59	6.71
LLCM2	-1.545	2.08	93.3	67	6.71
LSEM1	-1.528	2.09	93.3	67	6.70
LSEM2	-1.544	2.08	93.1	69	6.71
GAPI	-0.295	2.16	93.9	61	4.74
Bollen	-0.304	2.18	98.2	18	4.85
REG1	-1.535	2.12	93.8	62	6.85
REG2	-0.128	2.17	95.6	44	4.71
NoCov	1.934	4.16	22.1	0	7.58

Table 4.2 with Quadratic, Normal, $n_1 = 50$, $n_2 = 50$, $\gamma_1 = 2$

Method	Bias	Ave. Std. Err.	CI coverage	Power	MSE
NLCM1	-0.031	1.63	96.1	223	2.67
NLCM2	-0.040	1.63	95.8	227	2.64
LLCM1	-0.418	1.61	98.4	78	2.76
LLCM2	-0.421	1.60	98.2	81	2.75
LSEM1	-0.372	1.62	98.1	88	2.77
LSEM2	-0.417	1.61	98.1	84	2.76
GAPI	-0.093	1.65	95.7	210	2.72
Bollen	-0.118	1.67	98.8	77	2.79
REG1	-0.422	1.64	98.1	78	2.86
REG2	-0.034	1.69	96.0	210	2.85
NoCov	1.326	3.59	19.4	0	9.27

Table 4.3 with Quadratic, Normal, $n_1 = 100$, $n_2 = 200$, $\gamma_1 = 2$

Method	Bias	Ave. Std. Err.	CI coverage	Power	MSE
NLCM1	-0.097	1.03	93.8	438	1.07
NLCM2	-0.106	1.02	93.8	438	1.06
LLCM1	-0.612	1.01	96.0	167	1.39
LLCM2	-0.615	1.01	96.0	170	1.39
LSEM1	-0.551	1.02	96.3	178	1.34
LSEM2	-0.612	1.01	96.0	170	1.39
GAPI	-0.160	1.04	94.2	405	1.12
Bollen	-0.183	1.07	98.7	239	1.18
REG1	-0.615	1.02	96.2	163	1.42
REG2	-0.101	1.05	93.7	424	1.10
NoCov	1.932	2.26	4.7	0	5.10

Table 4.4 with Quadratic, Chi Square, $n_1 = 50$, $n_2 = 50$, $\gamma_1 = 1$

Method	Bias	Ave. Std. Err.	CI coverage	Power	MSE
NLCM1	-0.046	2.00	95.9	62	4.01
NLCM2	-0.060	1.97	95.8	63	3.90
LLCM1	1.769	2.07	96.4	95	7.40
LLCM2	1.759	2.06	95.9	102	7.33
LSEM1	1.860	2.08	95.4	108	7.79
LSEM2	1.772	2.07	95.6	102	7.42
GAPI	0.079	2.06	95.4	72	4.23
Bollen	0.002	2.10	98.6	26	4.41
REG1	1.799	2.13	95.5	94	7.77
REG2	-0.056	2.07	96.1	66	4.28
NoCov	1.227	6.53	81.0	0	4.06

Table 4.5 with Quadratic, Chi Square, $n_1 = 100$, $n_2 = 200$, $\gamma_1 = 2$

Method	Bias	Ave. Std. Err.	CI coverage	Power	MSE
NLCM1	-0.087	1.28	94.5	309	1.66
NLCM2	-0.094	1.28	94.4	309	1.65
LLCM1	-0.274	1.31	98.3	128	1.78
LLCM2	-0.280	1.30	98.3	130	1.77
LSEM1	-0.175	1.31	98.4	148	1.76
LSEM2	-0.273	1.31	98.2	132	1.78
GAPI	-0.114	1.32	94.9	284	1.75
Bollen	-0.136	1.31	98.0	174	1.83
REG1	-0.281	1.31	98.2	125	1.81
REG2	-0.102	1.29	94.8	291	1.68
NoCov	3.127	3.41	45.0	0	2.18

Table 4.6 with Quadratic, Gamma, $n_1 = 50$, $n_2 = 50$, $\gamma_1 = 0$

Method	Bias	Ave. Std. Err.	CI coverage	Power	MSE
NLCM1	-0.049	2.01	94.5	55	4.06
NLCM2	-0.049	2.01	94.4	56	4.03
LLCM1	-0.315	2.03	96.0	40	4.21
LLCM2	-0.315	2.03	95.7	43	4.20
LSEM1	-0.303	2.04	95.5	45	4.25
LSEM2	-0.312	2.03	95.6	44	4.20
GAPI	-0.080	2.04	94.5	55	4.15
Bollen	-0.080	2.09	97.6	24	4.36
REG1	-0.307	2.07	95.8	42	4.37
REG2	-0.029	2.07	94.7	53	4.28
NoCov	-0.566	4.78	68.7	0	3.65

Table 4.7 with Quadratic, Gamma, $n_1 = 50$, $n_2 = 50$, $\gamma_1 = 2$

Method	Bias	Ave. Std. Err.	CI coverage	Power	MSE
NLCM1	-0.034	1.97	96.3	154	3.87
NLCM2	-0.058	1.94	96.0	161	3.78
LLCM1	0.407	2.01	97.7	116	4.20
LLCM2	0.383	1.99	97.7	121	4.10
LSEM1	0.557	2.02	97.5	152	4.40
LSEM2	0.414	2.01	97.6	130	4.21
GAPI	0.035	2.00	94.8	169	4.02
Bollen	-0.017	2.04	98.7	74	4.15
REG1	0.416	2.05	97.6	122	4.38
REG2	-0.031	2.05	95.3	153	4.20
NoCov	3.614	5.01	72.5	0	3.46

Table 4.8 with Quadratic, Gamma, $n_1 = 100$, $n_2 = 200$, $\gamma_1 = 1$

Method	Bias	Ave. Std. Err.	CI coverage	Power	MSE
NLCM1	-0.058	1.21	94.8	120	1.47
NLCM2	-0.061	1.21	94.8	122	1.46
LLCM1	-0.854	1.26	96.5	13	2.32
LLCM2	-0.854	1.26	96.4	13	2.32
LSEM1	-0.789	1.27	96.6	17	2.24
LSEM2	-0.854	1.26	96.4	13	2.32
GAPI	-0.119	1.25	95.0	111	1.57
Bollen	-0.126	1.27	98.2	51	1.62
REG1	-0.861	1.26	96.4	16	2.34
REG2	-0.068	1.23	94.4	120	1.51
NoCov	0.291	3.06	46.1	0	1.40

Table 4.9 with Linear, Normal, $n_1 = 50$, $n_2 = 50$, $\gamma_1 = 1$

Method	Bias	Ave. Std. Err.	CI coverage	Power	MSE
NLCM1	0.061	2.47	94.8	77	6.08
NLCM2	-0.001	2.32	95.4	71	5.38
LLCM1	-0.035	2.38	94.9	74	5.67
LLCM2	-0.035	2.38	94.8	77	5.65
LSEM1	-0.097	2.41	94.4	78	5.79
LSEM2	-0.040	2.38	94.4	81	5.69
GAPI	0.036	2.45	93.9	90	6.00
Bollen	0.116	2.53	98.6	32	6.40
REG1	-0.059	2.44	94.7	73	5.95
REG2	0.020	2.54	94.5	70	6.47
NoCov	-1.169	5.15	30.0	0	14.66

Table 4.10 with Linear, Chi Square, $n_1 = 100$, $n_2 = 200$, $\gamma_1 = 2$

Method	Bias	Ave. Std. Err.	CI coverage	Power	MSE
NLCM1	0.006	1.46	95.8	289	2.13
NLCM2	-0.012	1.45	95.7	288	2.09
LLCM1	-0.133	1.45	95.5	259	2.13
LLCM2	-0.135	1.45	95.4	262	2.13
LSEM1	-0.058	1.47	95.1	276	2.16
LSEM2	-0.133	1.46	95.4	266	2.13
GAPI	-0.009	1.46	95.7	295	2.13
Bollen	0.006	1.48	99.0	141	2.18
REG1	-0.137	1.46	95.1	247	2.15
REG2	-0.003	1.47	95.5	271	2.15
NoCov	1.390	2.88	7.0	0	8.63

Table 4.11 with Linear, Gamma, $n_1 = 50$, $n_2 = 50$, $\gamma_1 = 1$

Method	Bias	Ave. Std. Err.	CI coverage	Power	MSE
NLCM1	0.114	2.44	95.1	63	5.96
NLCM2	0.010	2.21	95.7	54	4.88
LLCM1	0.448	2.39	94.2	90	5.92
LLCM2	0.392	2.29	94.8	85	5.39
LSEM1	-0.040	2.42	94.6	67	5.84
LSEM2	0.437	2.39	93.4	102	5.89
GAPI	0.150	2.43	93.7	96	5.94
Bollen	0.258	2.50	98.4	28	6.30
REG1	0.449	2.40	95.1	78	5.95
REG2	0.091	2.48	95.3	58	6.16
NoCov	-10.034	5.05	0.0	719	149.33

5. Example

This section presents an application of the latent covariate method estimation procedure to data from a substance abuse prevention study at the Institute for Social and Behavioral Research at Iowa State University. (See the following website for project information. http://www.projectfamily.isbr.iastate.edu.) The program was introduced to Iowa families with a child in the 6th grade. The behavioral measures used in this example

include self-reported levels of parenting behaviors and adolescent substance use, problem behaviors, and peer relations. The study followed each family in a longitudinal study. We will compare the treatment group that participated in the Preparing For the Drug Free Years (PDFY) program, a five session Life Skills Training, to a minimal-contact control group. We have used parent responses at pre-intervention for the covariate, which should be independent of treatment effect, and 8th grade post-intervention measurements on the adolescents for the response. Based on theoretical considerations and past experience with these measures, we would expect a nonlinear relationship between positive parenting skills and negative adolescent behaviors. This pattern is faintly shown in Figure 1.

The latent construct used for problem behaviors in children has six indicators: gateway substance use (GSUI), school-related problem behaviors (SRPB), behavioral tendency toward alcohol use (BTTAU), child self-restraint (CHSR), cross-setting oppositional behaviors (CSOB), and affiliation with antisocial peers (AFPP). The substance use index is a sum of 4 yes/no responses for various substances, scored so that higher values represent a higher level of substance use. Cross-setting oppositional behaviors consist of seven items involving anger, arguing, and disobedience and are measured on a seven-point Likert-type scale with the items averaged. High scores represent higher levels of problem behaviors. The remaining indicators cover a variety of problem behaviors related to skipping school, stealing, fighting, arguing, and similar issues including those regarding the behavior of their closest friends, all of which are measured on a five-point Likert-type scale and averaged for each indictor grouping. High scores of these measures indicate higher levels of problem behaviors. The alpha reliabilities for the items contained in each of the problem behavior scale measures ranged between 0.70 and 0.89.

The latent construct used for parenting behaviors has seven indicators: intervention targeted parenting behaviors (ITPB), affective quality (AQ), general child management (GCM), recurring conflicts (RECF), parental externalizing (PASR), marital stability (MRST), and spouse problem behaviors (SPB). The intervention targeted parenting behaviors scale consists of fourteen items scaled on a five-point Likert-type scale and averaged. Affective quality is measured with the average of seven items scaled on a seven point Likert-type scale. Recurring conflicts is measured as the average of three items scaled on a seven point Likert-type scale. General child management is the average of thirteen items scaled on a seven point Likert-type scale. Parental externalizing is the average of six items and spouse problem behaviors is also the average of six items, both scaled on a five point Likert-type scale. Marital stability is measured as the average of five items scaled on a four point Likert-type scale. High scores of these measures indicate better parenting skills. The alpha reliabilities for the items contained in each of the parenting behavior scale measures ranged between 0.70 and 0.88.

We fit the following measurement model using a selected subset of the data where we had responses available from both targets and parents at both time periods.

$$x_{ij} = \begin{pmatrix} ITPB \\ AQ \\ RECF \\ PASR \\ MRST \\ SPB \\ GCM \end{pmatrix} = \begin{pmatrix} \beta_{01} \\ \beta_{02} \\ \beta_{03} \\ \beta_{04} \\ \beta_{05} \\ \beta_{06} \\ 0 \end{pmatrix} + \begin{pmatrix} \beta_{11} \\ \beta_{12} \\ \beta_{13} \\ \beta_{14} \\ \beta_{15} \\ \beta_{16} \\ 1 \end{pmatrix} f_{ij} + \varepsilon_{xij},$$

where $i = 0,1$ and $j = 1,2,\ldots,n_i$ and where $n_0 = 83$ and $n_1 = 89$. We also fit values for y_{ij} with the following model

$$y_{ij} = \begin{pmatrix} GSUI \\ BTTAU \\ CHSR \\ AFPP \\ CSOB \\ SRPB \end{pmatrix} = \begin{pmatrix} \alpha_{01} \\ \alpha_{02} \\ \alpha_{03} \\ \alpha_{04} \\ \alpha_{05} \\ 0 \end{pmatrix} + \begin{pmatrix} \alpha_{11} \\ \alpha_{12} \\ \alpha_{13} \\ \alpha_{14} \\ \alpha_{15} \\ 1 \end{pmatrix} g_{ij} + \varepsilon_{yij}.$$

We examine scatter plots of $\hat{g}_{ij} - \bar{\hat{g}}_{i\cdot}$ vs. $\hat{f}_{ij} - \bar{\hat{f}}_{i\cdot}$ (Pictured in Figure 2) and $\hat{g}_{ij} - \bar{\hat{g}}_{i\cdot}$ vs. $\left(\hat{f}_{ij} - \bar{\hat{f}}_{i\cdot}\right)^2$ (Pictured in Figure 3) to provide insight into what functional form of the covariate relationship might be appropriate for this data. Looking at Figure 2, we see that the scatter plot possibly shows a slightly curved pattern and in Figure 3, the pattern is close to random in appearance. This, along with the scatter plot in Figure 1 and mainly from theoretical considerations of behavioral patterns, leads us toward a quadratic model. From the model (1.1), we have that

$$g_{ij} = \mu_i + \zeta_{ij}, \quad \text{i} = 1,2 \text{ and } \text{j} = 1,\ldots, n_i,$$

and we decided on the following nonlinear quadratic structured model

$$h\left(f_{ij};\gamma\right) = \gamma_0 + \gamma_1 D_i + \gamma_2 f_{ij} + \gamma_3 f_{ij}^2, \tag{5.1}$$

where D_i is the dichotomized treatment variable.

The latent covariate method with the nonlinear structural model, NLCM2, indicated that the intervention parameter γ_1 in (5.1) is close to significant with a p-value of 0.05989. The linear SEM (LSEM) also did not find the intervention to be significant with a larger p-value of 0.06902. Simple regression with latent covariate terms treated as explanatory variables also did not find the intervention to be significant with an even larger p-value of 0.08812. This represents one possible instance where ignoring the nonlinearity inherent in

the relationships of the latent structures may cause a researcher to miss important differences. This may be the case even though simply looking at a graph of the data, as shown in Figure 1, might not suggest a difference between intervention and control groups.

In conclusion, we have indeed presented a sound and easily applicable method of assessing intervention effects for experimental studies where the treatment groups are appropriately randomly assigned and most of the conceptual variables are indirectly measured. The latent covariate method provides a useful and coherent analysis of covariance procedure with a reliable and practical way to incorporate nonlinear covariates.

Figure 1: Family Measures

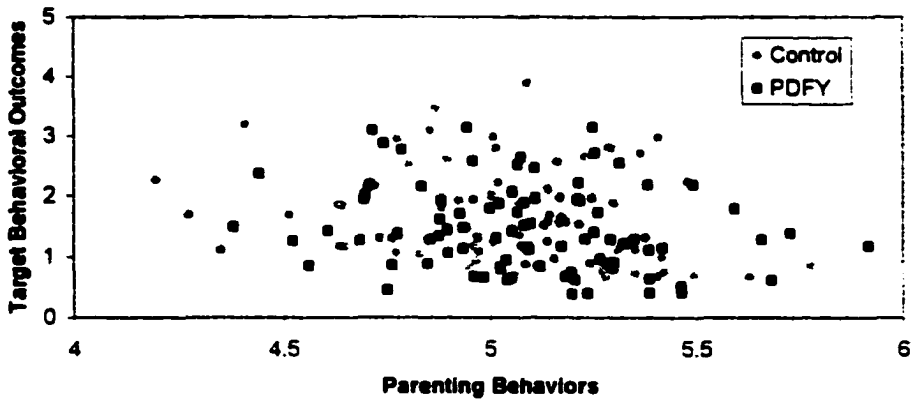


Figure 2: Diagnostic Scatter Plot

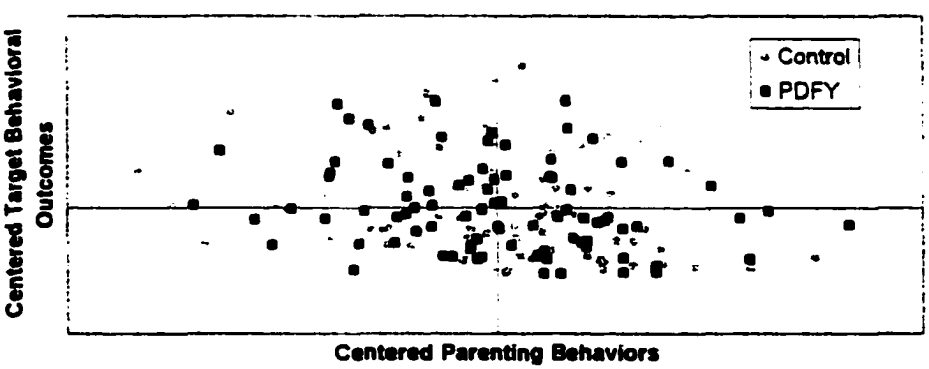
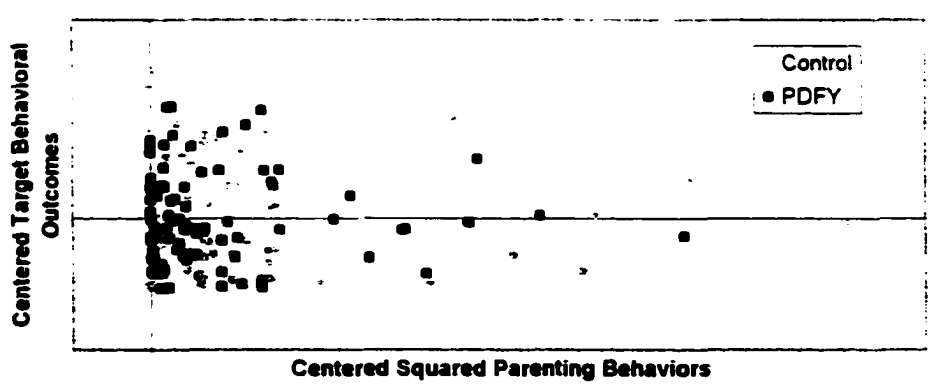


Figure 3: Diagnostic Scatter Plot



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IMPROVED INFERENCE PROCEDURES FOR TRUE VALUES OF LATENT VARIABLES

A paper to be submitted to Biometrika

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Abstract

The use of latent factor structure is reasonable in social, medical, business, and behavioral sciences because the theoretical constructs are often observed only indirectly through a set of observable indicators. Although estimates of standard factor scores are available, making inferences about the true value of a latent construct has not been discussed widely. In this paper, a variance estimator for the factor score estimator is derived that incorporates the additional variability due to the parameter estimation. Also, an estimated residual vector in the latent variable analysis is defined, and its properties derived.

Diagnostic procedures using the factor score and residual estimates are proposed. Simulation studies and an example are given.

1. Introduction

Factor analysis and structural equation modeling are commonly used in many disciplines including social, medical, business, and behavioral sciences. The use of latent factor structure is reasonable in these research areas because the variables of primary interest are mainly theoretical constructs that are often observed only indirectly through a set of observable indicators. Estimation of the true latent variable values should be of interest in many applications, but has not been fully discussed from a statistical point of view. In factor analysis, an often considered estimator of the true, unobservable factor value is the so-called Bartlett's factor score estimator. See, e.g., Lawley and Maxwell (1963), Bollen (1989) and Fuller (1987). Although this estimator, which treats the factors as fixed constants, has intuitive appeal, it has limited inference and diagnostic uses. The estimator is a type of regression or generalized least squares estimator based on the fitted or estimated model. Thus, the variability in the estimator is large for two reasons. First, the individual-specific factor score estimator depends largely on observations from this particular individual, and the estimation error does not vanish even with infinitely many individual observations. Second, variability in factor score estimation includes errors due to the estimation of the model parameters. Thus, it should be important to capture the contribution of this estimation error, which depends on the sample size and which gives correlation among factor score estimators for different individuals.

In this paper, we derive an estimated variance for the factor score estimator that incorporates parameter estimation variability. The use of such a variance estimator for inferences about the true score values and for diagnostic purposes is discussed. In conjunction with the factor score estimation, we define an estimated residual and propose how it can be used in model diagnostics. We note that any linear structural equation model consisting of both a measurement model and a structural model can be expressed as a special case of the factor analysis model. For this reason, and for simplicity, we present our development only in terms of the basic factor analysis model in this paper. We utilize the expansion form given in Wall and Amemiya (2000) to introduce a factor score estimator for polynomial structural equation models.

Let a p-dimensional vector of observations on the t^{th} individual be denoted by

$$Z_t = \left(Z_{t1}, Z_{t2}, \ldots, Z_{tp}\right)', \qquad t = 1,2,\ldots,n.$$

It is assumed that the vector can be expressed as the sum of a linear function of an unobservable factor vector $f_t\,(k \times 1)$ and an error vector $\varepsilon_t\,(p \times 1)$. To discuss the true value of the factor, the factor vector needs to be uniquely defined and identified. The standard identified factor analysis model uses the errors-in-variable parameterization that places zero/one restriction on coefficients but leaves factors unrestricted. For this parameterization, after possible re-ordering of the elements of Z_t, we divide $Z_t\ (p \times 1)$ into two parts,

$Z_t = \left(y_t', x_t'\right)'$ with $y_t\ (p-k) \times 1$ and $x_t\ (k \times 1)$, and the factor analysis model as

$$Z_t = \begin{pmatrix} y_t \\ x_t \end{pmatrix} = \begin{pmatrix} \beta_0 \\ 0_{k\cdot 1} \end{pmatrix} + \begin{pmatrix} \beta_1 \\ I_k \end{pmatrix} f_t + \varepsilon_t, \qquad t = 1,\ldots,n, \tag{1.1}$$

where β_0 is $(p-k)\times 1$ and β_1 is $(p-k)\times k$ and for $\varepsilon_t = \begin{pmatrix} e_t \\ u_t \end{pmatrix}$, let $V\{\varepsilon_t\} = \Psi$. For simplicity, we will assume that Ψ is diagonal, although this is not necessary. The factor analysis model considered here is general in the sense that Ψ and β_1 can have any structure, but β_0 is assumed to be completely unknown. We assume that the model is identified in the sense that the unknown elements of β_0, β_1 and Ψ can be estimated from the first two sample moments. Since our interest is in estimating f_t without any specified distributional form, we treat f_t as fixed. We do not assume any distributional form for ε_t at this point.

To motivate factor score estimation, suppose that the parameters of model (1.1), β_0, β_1 and Ψ are given. Then, for each t we can apply generalized least squares estimation to

$$Z_t - \begin{pmatrix} \beta_0 \\ 0_{k\cdot 1} \end{pmatrix} = \begin{pmatrix} \beta_1 \\ I_k \end{pmatrix} f_t + \varepsilon_t$$

to obtain

$$\ddot{f}_t = \left[\left(\beta_1', I_k \right) \Psi^{-1} \begin{pmatrix} \beta_1 \\ I_k \end{pmatrix} \right]^{-1} \left(\beta_1', I_k \right) \Psi^{-1} \left[Z_t - \begin{pmatrix} \beta_0 \\ 0 \end{pmatrix} \right].$$

The alternative form not requiring the inverse of Ψ itself can be obtained as

$$\ddot{f}_t = x_t - \Gamma v_t, \tag{1.2}$$

where

$$\begin{aligned} v_t &= \left(I_{p-k}, -\beta_1 \right) \varepsilon_t \\ &= y_t - \beta_0 - \beta_1 x_t \\ &= e_t - \beta_1 u_t \end{aligned} \tag{1.3}$$

and

$$\Gamma = \Psi_{uv}\Psi_{vv}^{-1}. \tag{1.4}$$

where

$$\Psi_{uu} = \left(0_{k\times(p-k)}, I_k\right)\Psi\begin{pmatrix}0_{k\times(p-k)}\\ I_k\end{pmatrix},$$

$$\Psi_{vv} = \left(I_{p-k}, -\beta_1\right)\Psi\begin{pmatrix}I_{p-k}\\ -\beta_1'\end{pmatrix}, \tag{1.5}$$

and

$$\Psi_{uv} = \left(0_{k\times(p-k)}, I_k\right)\Psi\begin{pmatrix}I_{p-k}\\ -\beta_1'\end{pmatrix}. \tag{1.6}$$

Under model (1.1), $v_t = e_t - \beta_1 u_t$, which is free of f_t and has mean zero. Thus, this v_t can be considered a $(p-k)\times 1$ residual vector. We write $\ddot{f}_t$ as

$$\ddot{f}_t = f_t + r_t$$

where

$$r_t = \left(0_{k\times(p-k)}, I_k\right)\varepsilon_t - \Gamma v_t. \tag{1.7}$$

Then, the variance of r_t is

$$\Psi_{rr} = c\Psi c' = \Psi_{uu} - \Gamma\Psi_{vv}\Gamma' \tag{1.8}$$

where

$$c = \left(0_{k\times(p-k)}, I_k\right) - \Gamma\left(I_{p-k}, -\beta_1\right). \tag{1.9}$$

In practice, the model parameters are not known and need to be estimated. Let $\hat{\beta}_0$, $\hat{\beta}_1$ and $\hat{\Psi}$ denote the parameter estimators, e.g., obtained by the maximum likelihood under

the normality of f_t and ε_t. Under our assumption of unrestricted β_0 and unrestricted factor distribution,

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

where

$$\bar{y} = \frac{1}{n}\sum_{t=1}^{n} y_t \text{ and } \bar{x} = \frac{1}{n}\sum_{t=1}^{n} x_t . \tag{1.10}$$

Then, Bartlett's factor score estimator can be obtained by replacing β_0, β_1 and Ψ in (1.2) by $\hat{\beta}_0$, $\hat{\beta}_1$ and $\hat{\Psi}$, i.e.,

$$\hat{f}_t = x_t - \hat{\Gamma}\hat{v}_t , \tag{1.11}$$

where

$$\hat{\Gamma} = \hat{\Psi}_{uv}\hat{\Psi}_{vv}^{-1} \tag{1.12}$$

and

$$\hat{v}_t = e_t - \hat{\beta}_1 u_t , \tag{1.13}$$

where $\hat{\Gamma}$, $\hat{\Psi}_{uv}$, $\hat{\Psi}_{vv}$ and $\hat{v}_t$ are as in (1.4), (1.6), (1.5) and (1.3) with all parameters replaced by estimates $\hat{\beta}_0$, $\hat{\beta}_1$ and $\hat{\Psi}$.

If we write

$$\hat{f}_t = f_t + \hat{r}_t ,$$

then the variability in $\hat{r}_t$ includes the estimation error in the model parameter and is expected to be larger than Ψ_{rr} in (1.8). However, the standard estimator of $Var\left(\hat{f}_t\right)$ is

$$\hat{\Psi}_{rr} = \hat{c}\hat{\Psi}\hat{c}' = \hat{\Psi}_{uu} - \hat{\Gamma}\hat{\Psi}_{vv}\hat{\Gamma}' . \tag{1.14}$$

which estimates Ψ_r, but is expected to underestimate $Var\left(\hat{f}_t\right)$. Another deficiency of $\hat{\Psi}_r$ due to neglecting the parameter estimation error is that it is constant for all individuals, i.e., all t's. But, in practice, we should be able to estimate those f_t's near the middle of the data set, i.e., f_t's near the sample mean, with less error or variability than those very far away from a majority of the data points. In the next sections, we derive a new estimator of $Var\left(\hat{f}_t\right)$ incorporating the estimation error variability that turns out to depend on where the true f_t is located relative to the sample mean.

2. Asymptotic Expansions

To incorporate the variability due to the parameter estimation, we use an expansion of $\hat{f}_t - \ddot{f}_t$ in terms of the parameter estimators. Throughout the development in this section, we assume model (1.1) with associated assumptions, and derive asymptotic results as the sample size n tends to infinity. We also assume that the parameter estimators $\hat{\beta}_0$, $\hat{\beta}_1$ and $\hat{\Psi}$ have errors of order $n^{-1/2}$ in probability. From (1.11), we see that the parameter estimators enter $\hat{f}_t$ through $\hat{\Gamma}$ and $\hat{v}_t$. The first lemma gives an expansion of $\hat{\Gamma}$.

Lemma 1. For $\hat{\Gamma}$ and Γ defined in (1.12) and (1.4),

$$\hat{\Gamma} - \Gamma = c\left(\hat{\Psi} - \Psi\right)\begin{pmatrix} I_{p-k} \\ -\beta_1' \end{pmatrix}\Psi_w^{-1} - \Psi_r\left(\hat{\beta}_1 - \beta_1\right)'\Psi_w^{-1} + \Gamma\left(\hat{\beta}_1 - \beta_1\right)\Gamma + O_p\left(\frac{1}{n}\right),$$

where Ψ_w, c and Ψ_r are given in (1.5), (1.9) and (1.8).

Proof: Note that

$$\begin{aligned}\hat{\Gamma}-\Gamma &= \Psi_{uv}\Psi_{vv}^{-1}\left(\hat{\Psi}_{vv}-\Psi_{vv}\right)\Psi_{vv}^{-1}+\left(\hat{\Psi}_{uv}-\Psi_{uv}\right)\Psi_{vv}^{-1}+O_p\left(\frac{1}{n}\right) \\ &= \Gamma\left(\hat{\Psi}_{vv}-\Psi_{vv}\right)\Psi_{vv}^{-1}+\left(\hat{\Psi}_{uv}-\Psi_{uv}\right)\Psi_{vv}^{-1}+O_p\left(\frac{1}{n}\right)\end{aligned} \tag{2.1}$$

Meanwhile,

$$\hat{\Psi}_{uv}-\Psi_{uv}=\left(0_{k\times(p-k)},I_k\right)\left(\hat{\Psi}-\Psi\right)\begin{pmatrix}I_{p-k}\\-\beta_1'\end{pmatrix}+\left(0_{k\times(p-k)},I_k\right)\Psi\begin{pmatrix}0_{p-k}\\-\left(\hat{\beta}_1-\beta_1\right)'\end{pmatrix}$$

and

$$\begin{aligned}\hat{\Psi}_{vv}-\Psi_{vv} &= \left(I_{p-k},-\beta_1\right)\left(\hat{\Psi}-\Psi\right)\begin{pmatrix}I_{p-k}\\-\beta_1'\end{pmatrix} \\ &\quad +\left(0_{p-k},-\left(\hat{\beta}_1-\beta_1\right)\right)\Psi\begin{pmatrix}I_{p-k}\\-\beta_1'\end{pmatrix}+\left(I_{p-k},-\beta_1\right)\Psi\begin{pmatrix}0_{p-k}\\-\left(\hat{\beta}_1-\beta_1\right)'\end{pmatrix}.\end{aligned}$$

Substituting these into (2.1), we obtain

$$\begin{aligned}\hat{\Gamma}-\Gamma &= +c\left(\hat{\Psi}-\Psi\right)\begin{pmatrix}I_{p-k}\\-\beta_1'\end{pmatrix}\Psi_{vv}^{-1}+c\Psi\begin{pmatrix}0_{p-k}\\-\left(\hat{\beta}_1-\beta_1\right)'\end{pmatrix}\Psi_{vv}^{-1} \\ &\quad -\Gamma\left(0_{p-k},-\left(\hat{\beta}_1-\beta_1\right)\right)\Psi\begin{pmatrix}I_{p-k}\\-\beta_1'\end{pmatrix}\Psi_{vv}^{-1}+O_p\left(\frac{1}{n}\right)\end{aligned}$$

Since $c\Psi\left(0_{k\times(p-k)},I_k\right)'=\Psi_{rr}$, and since $\left(0_{k\times(p-k)},I_k\right)\Psi\left(I_{p-k},-\beta_1\right)'=\Psi_{uv}$, the result follows.

□

The next lemma gives an expansion of $\hat{f}_t-\ddot{f}_t$ in terms of $\hat{\Gamma}-\Gamma$.

Lemma 2. For $\hat{f}_t$ in (1.11) and $\ddot{f}_t$ in (1.2),

$$\hat{f}_t - \ddot{f}_t = \Gamma\left[\bar{v} + \left(\hat{\beta}_1 - \beta_1\right)\left(x_t - \bar{x}\right)\right] - \left(\hat{\Gamma} - \Gamma\right)v_t + O_p\left(\frac{1}{n}\right)$$

where $\bar{v} = \bar{e} - \beta_1\bar{u}$, with v_t from (1.3), Γ from (1.4) and $\hat{\Gamma}$ from (1.12).

Proof: Note that

$$\begin{aligned} \hat{v}_t - v_t &= y_t - \bar{y} - \hat{\beta}_1\left(x_t - \bar{x}\right) - v_t \\ &= -\left(\hat{\beta}_1 - \beta_1\right)\left(x_t - \bar{x}\right) - \bar{v} \end{aligned} \tag{2.2}$$

Thus,

$$\begin{aligned} \hat{f}_t - \ddot{f}_t &= \Gamma v_t - \hat{\Gamma}\hat{v}_t \\ &= -\left(\hat{\Gamma} - \Gamma\right)v_t - \Gamma\left(\hat{v}_t - v_t\right) + O_p\left(\frac{1}{n}\right), \end{aligned}$$

and the result follows. □

The next theorem gives the expansion of $\hat{f}_t - f_t$ up to terms of order $n^{-1/2}$.

Theorem 1. The factor score estimator $\hat{f}_t$ in (1.11) satisfies

$$\begin{aligned} \hat{f}_t - f_t = r_t + \Gamma\bar{v} &- \left[v_t'\Psi_{ww}^{-1}\left(I_{p-k}, -\beta_1\right)\otimes c\right]vec\left(\hat{\Psi} - \Psi\right) \\ &+ \left\{\left[\left(\ddot{f}_t - \bar{f}\right)'\otimes\Gamma\right] + \left[v_t'\Psi_{ww}^{-1}\otimes\Psi_{rr}\right]\mathrm{P}\right\}vec\left(\hat{\beta}_1 - \beta_1\right) + O_p\left(\frac{1}{n}\right), \end{aligned}$$

where r_t is given in (1.7), $\bar{f} = \bar{x} - \Gamma\bar{v}$, $\otimes$ is the Kronecker product and P is a matrix such that $PvecD' = vecD$ for any matrix D.

Proof: Note that for any conforming matrices A, B, and C, $vec(ABC) = (C'\otimes A)vecB$. Using this, Lemmas 1 and 2, $\ddot{f}_t = x_t - \Gamma v_t$ and $\bar{x} - \bar{f} = O_p\left(n^{-1/2}\right)$, we can derive the result after some algebra. □

For the estimated residual $\hat{v}_t$ in (1.13), we have the following expression.

Theorem 2. The estimated residual vector $\hat{v}_t$ satisfies

$$\hat{v}_t = v_t - \bar{v} - \left(\hat{\beta}_1 - \beta_1\right)\left(\Gamma v_t + \ddot{f}_t - \bar{f}\right) + O_p\left(n^{-1}\right)$$

Proof: Applying the arguments used in the proof of Theorem 1 to (2.2), we obtain the result. □

3. Approximate variances and covariances and their use in diagnostics

The asymptotic expansions given in the previous section can be used to obtain inference procedures related to the true value of f_t and the residual v_t. The expansions in Theorems 1 and 2 are valid for any distribution of ε_t. However, to obtain a relatively simple form of an estimated variance, we assume that all third moments of ε_t are zero. This assumption is weaker than either a symmetric distribution around zero or normality. However, for inference statements such as confidence interval results, we act as though the error ε_t is normally distributed. The distribution of the true factor values, the f_t's, is assumed totally unknown and unspecified, and the f_t's are treated as fixed. We also assume that the leading terms in the asymptotic distributions of $\hat{\Psi}$ and $\hat{\beta}_1$ are quadratic functions of ε_t. This is in fact true for any estimator based on the sample covariance matrix. The factor analysis model considered here is general in the sense that Ψ and β_1 can have any structure. To express this general form, we write Ψ and β_1 as functions of a parameter θ; $\Psi = \Psi(\theta)$

and $\beta_1 = \beta_1(\theta)$. We assume that the derivative of these functions exist, so that the usual delta method expansion of $\hat{\Psi}$ and $\hat{\beta}_1$ around $\hat{\theta}$ can be written as

$$vec\hat{\Psi} = L_\psi\left(\hat{\theta} - \theta\right) + o_p\left(n^{-1}\right),$$

$$vec\hat{\beta}_1 = L_\beta\left(\hat{\theta} - \theta\right) + o_p\left(n^{-1}\right)$$

and that $\hat{L}_\psi$ and $\hat{L}_\beta$ denote consistent estimators of L_ψ and L_β. If the structure of Ψ and β_1 allow only known elements and equality constraints, L_ψ and L_β are constants and need not be estimated. Let $\hat{\Omega}$ denote an estimated covariance matrix of $\hat{\theta}$. We should point out that, for the normal maximum likelihood or related estimator $\hat{\theta}$, the standard $\hat{\Omega}$ is valid for any unspecified distribution of f_t (or fixed). See, e.g., Amemiya, Fuller, and Pantula (1987), Anderson and Amemiya (1987), and Browne and Shapiro (1987). Throughout, we attempt to obtain a variance estimator by considering terms in an expansion up to $O_p\left(n^{-1/2}\right)$, which corresponds to variance terms up to $O\left(n^{-1}\right)$.

As an estimator of the covariance matrix of $\hat{f}_t - f_t$ based on the expansion in Theorem 1, we propose the use of

$$\hat{V}_t = \hat{\Psi}_{rr} + \frac{1}{n}\hat{\Gamma}\hat{\Psi}_{ww}\hat{\Gamma}' + A_t\hat{\Omega}A_t', \tag{3.1}$$

where $\hat{\Psi}_{rr}$, $\hat{\Gamma}$ and $\hat{\Psi}_{ww}$ are given in (1.14), (1.12) and (1.5), $\hat{\Omega}$ is the estimated covariance matrix of $\hat{\theta}$,

$$A_t = \left[\left(\hat{f}_t - \bar{x}\right)' \otimes \hat{\Gamma}\right]\hat{L}_\beta + \left[\left(\hat{v}_t'\hat{\Psi}_{ww}^{-1} \otimes I_k\right)\left(I_{p-k} \otimes \hat{\Psi}_{rr}\right)\right]P\hat{L}_\beta - \left[\left(I_{p-k}, \hat{\beta}_1\right) \otimes \hat{c}\right]\hat{L}_\psi,$$

and $\hat{f}_t$, $\hat{v}_t$, $\bar{x}$ and P are defined in (1.11), (1.13), (1.10) and Theorem 1. In this estimator, we used $\hat{f}_t$, $\hat{v}_t$ and $\bar{x}$ to estimate $\ddot{f}_t$, v_t and $\bar{f}$ appearing in Theorem 1. As a result, this formula is individual specific, i.e., depends on t. In particular, the variance estimator depends on the location of the individual relative to the center, i.e., $\hat{f}_t - \bar{x}$, and on how the individual deviates from the fitted model, i.e., the estimated residual $\hat{v}_t$. The form (3.1) clearly indicates that the estimated variance is the estimated variance $\hat{\Psi}_{rr}$ for $\ddot{f}_t$ plus an additional variability due to $\hat{\theta}$ estimation, and that this additional variability depends on the individual. For constructing a 95% confidence interval for the true latent variable value f_t, we suggest the use of $\hat{f}_t \pm 1.96\sqrt{\hat{V}_t}$.

If we wish to compare the true factor values of two individuals t and s, we need an estimated variance for the estimated difference $\hat{f}_t - \hat{f}_s$, $t \neq s$. Note that, in applying the expansion of Theorem 1 to $\hat{f}_t - \hat{f}_s$, the $\Gamma\bar{v}$ terms cancel out. Thus, an estimated covariance matrix of the estimated difference $\hat{f}_t - \hat{f}_s$ is

$$\hat{D}_{ts} = 2\hat{\Psi}_{rr} + (A_t - A_s)\hat{\Omega}(A_t - A_s)'. \tag{3.2}$$

Using this, we can, e.g., perform a test comparing two individual true values (equality or inequality).

One use of $\hat{f}_t$ and $\hat{v}_t$ is for diagnostic purposes. In latent variable analysis, an individual can be considered unusual or outlying for two different reasons. An unobservable individual characteristic f_t can be away from the majority or the middle part of the population. Alternatively, the proposed model may not fit observed measurements with large

random errors from a particular individual. These two types of outliers can be assessed using $\hat{f}_t$ and $\hat{v}_t$, respectively. To discuss possibly unusual f_t, we need to specify the distribution of f_t. If the population distribution of f_t can be treated as normal, we can test whether an individual t has an unusual characteristic f_t by comparing

$$\left(\hat{f}_t - \bar{x}\right)' \left(\hat{\phi} + \hat{V}_t\right)^{-1} \left(\hat{f}_t - \bar{x}\right) \tag{3.3}$$

to a chi-square (with degrees of freedom k) cut-off point with $\hat{\phi}$ being an estimated variance of f_t from the factor analysis fit. Or, a test can be performed component-wise using a normality-based cut-off point. To assess an individual deviation from the model, without assuming any distribution for f_t, we can compare

$$\hat{v}_t' \hat{H}_t \hat{v}_t \tag{3.4}$$

to a chi-square (with degrees of freedom $p-k$) cut-off point, where $\hat{H}_t$ is an estimated covariance matrix of $\hat{v}_t$ based on Theorem 2,

$$\hat{H}_t = \left(1 - \frac{1}{n}\right) \hat{\Psi}_w + B_t \hat{\Omega} B_t',$$

$$B_t = \left[\left(\hat{\Gamma}\hat{v}_t + \hat{f}_t - \bar{x}\right)' \otimes I_{p-k}\right] \hat{L}_\beta .$$

4. Simulation Studies

A simulation study was conducted to show the differences in the variance estimates of the latent variable when the variability due to the estimation of θ is incorporated. The

following are results from sets of simulated data. The model was simulated using 4 different sample sizes (n=25, 50, 100, and 200) and using 3 different distributions for the latent factor (normal, chi-square, and uniform). Thus, there are 12 different situations. 1000 samples were generated for each situation. For each distribution, 5 values were chosen for f_t representing one value close to the mean, a pair of values roughly 2 standard deviations on either side of the mean, and another pair of values roughly 3 standard deviations on either side of the mean. The mean empirical variance is given as the mean of the variances of the estimates of f_t. The variance of $\hat{f}_t$ is estimated in two ways. The mean of each of the 1000 $\hat{\Psi}_{rr}$'s from (1.14) values are included and the mean of the 1000 $\hat{V}_t$'s from (3.1) were calculated along with coverages for 95% confidence intervals. The results are presented in Tables 4.1 through 4.12.

The measurement model and parameter values used were

$$\begin{pmatrix} z_{1t} \\ z_{2t} \\ z_{3t} \\ z_{4t} \\ z_{5t} \\ z_{6t} \end{pmatrix} = \begin{pmatrix} 0.3 \\ 0.1 \\ -0.2 \\ 0.05 \\ -0.05 \\ 0 \end{pmatrix} + \begin{pmatrix} 1.3 \\ 0.8 \\ 1.1 \\ 0.9 \\ 1.2 \\ 1.0 \end{pmatrix} f_t + \begin{pmatrix} \varepsilon_{1t} \\ \varepsilon_{2t} \\ \varepsilon_{3t} \\ \varepsilon_{4t} \\ \varepsilon_{5t} \\ \varepsilon_{6t} \end{pmatrix}, \quad t = 1,\ldots,n, \tag{4.1}$$

where the different latent factor distributions were $f_t \sim N(10,3), \chi^2_4, Unif(2,8)$, and the errors were generated standard normal and independently of f_t.

We conclude that without a doubt, the variance estimate $\hat{V}_t$ is much closer to the empirical variance estimate. The standard variance method, $\hat{\Psi}_{rr}$, consistently underestimates the empirical variance. Also, the 95% confidence interval coverages using $\hat{V}_t$

are considerably closer to the targeted 95%, particularly for non-normal data, smaller sample sizes, and values away from the mean, such as the 2 and 3 standard deviations from the mean than when using $\hat{\Psi}_{\pi}$.

A second set of simulations was conducted to illustrate how $\hat{f}_t$ and $\hat{v}_t$ can be used to assess the two different types of outliers. For simplicity, we will refer to each of the statistics used to detect outliers by κ_1, κ_2 and κ_3. A basic way to assess outliers may be to use

$$\kappa_1 = (Z_t - \bar{Z})' \hat{V}(Z_t)^{-1} (Z_t - \bar{Z}), \tag{4.2}$$

where Z_t are the data from (4.1) and $\hat{V}(Z_t)$ is the basic standard estimate of variance of a vector of observations. However, this approach leaves us unable to assess the type of outlier and does not take into account the variability due to the estimation of the parameters. As stated in Section 3, we can test whether an individual has an unusual characteristic f_t with the formula from (3.3),

$$\kappa_2 = (\hat{f}_t - \bar{x})' (\hat{\phi} + \hat{V}_t)^{-1} (\hat{f}_t - \bar{x}) \tag{4.3}$$

and we can test whether an individual deviates from the model with a large residual, v_t, with the formula from (3.4),

$$\kappa_3 = \hat{v}_t' \hat{H}_t \hat{v}_t. \tag{4.4}$$

The following are results from a set of simulated data that contain outliers of both types and an outlier that has both a large f_t and a large residual, v_t. The model and parameter values used were

$$\begin{pmatrix} z_{1t} \\ z_{2t} \\ z_{3t} \\ z_{4t} \\ z_{5t} \end{pmatrix} = \begin{pmatrix} -.03 \\ .1 \\ -.14 \\ .05 \\ 0 \end{pmatrix} + \begin{pmatrix} 1.15 \\ .86 \\ 1.05 \\ .92 \\ 1 \end{pmatrix} f_t + \begin{pmatrix} \varepsilon_{1t} \\ \varepsilon_{2t} \\ \varepsilon_{3t} \\ \varepsilon_{4t} \\ \varepsilon_{5t} \end{pmatrix}, \qquad t = 1,\ldots,100,$$

where $f_t \sim N(5,1)$, $\varepsilon_t \sim N(0,1)$, and the errors were generated independently of f_t. The outlier caused by a large latent variable factor had a value of 4.5 added to f_t. The outlier caused by a large v_t had a value of 7.84 added to z_{1t}. The outlier caused by both a large latent factor and a large residual, v_t, had a value of 4.0 added to f_t and a value of 5.76 added to z_{1t}. To assess for the existence of outliers, κ_1 (4.2) divided by 4 was compared to an F with (5,99) df., κ_2 (4.3) was compared to an F with (1,99) df, and κ_3 (4.4) divided by 4 was compared to an F with (4,99) df. The results are presented in Table 4.13. A second simulation was run with the exact same model except the latent factor was generated as a Chi-Square with 6 df that was standardized and shifted to (4,1). The results are presented in Table 4.14.

In both cases, κ_1 (4.2) was unable to provide any insight into the cause of the outlier. Also, κ_2 (4.3) and κ_3 (4.4) correctly distinguished the observations that were caused by each type of outlier.

As we have shown, failing to incorporate the additional variability due to parameter estimation makes a big difference in inferences and accuracy of testing procedures. This includes inability to correctly recognize outliers and also results in too small coverage probabilities for confidence intervals. This extends even to larger sample sizes, where the adjustment in variance estimate also makes an impact in inference.

Table 4.1. Normal(10,3) with n=25

	True value	3	6	10	14	17
	Empirical variance	0.306	0.229	0.194	0.221	0.266
ave. est.	$\hat{\Psi}_{rr}$	0.124	0.124	0.124	0.124	0.124
variance	$\hat{V}_t$	0.265	0.200	0.169	0.197	0.259
95% CI	$\hat{\Psi}_{rr}$	77.8	85.5	88.2	84.6	80.2
coverage	$\hat{V}_t$	92.7	93.2	93.0	93.0	94.7

Table 4.2. Normal(10,3) with n=50

	True value	3	6	10	14	17
	Empirical variance	0.233	0.180	0.174	0.187	0.246
ave. est.	$\hat{\Psi}_{rr}$	0.136	0.136	0.136	0.136	0.136
variance	$\hat{V}_t$	0.218	0.178	0.159	0.182	0.227
95% CI	$\hat{\Psi}_{rr}$	85.6	90.6	92.0	90.0	85.3
coverage	$\hat{V}_t$	94.0	94.4	94.1	94.5	94.4

Table 4.3. Normal(10,3) with n=100

	True value	3	6	10	14	17
	Empirical variance	0.313	0.200	0.164	0.210	0.288
ave. est.	$\hat{\Psi}_{rr}$	0.141	0.141	0.141	0.141	0.141
variance	$\hat{V}_t$	0.201	0.169	0.153	0.167	0.196
95% CI	$\hat{\Psi}_{rr}$	89.2	93.0	93.3	90.8	89.9
coverage	$\hat{V}_t$	94.2	95.4	94.6	93.4	94.6

Table 4.4. Normal(10,3) with n=200

	True value	3	6	10	14	17
	Empirical variance	0.188	0.169	0.155	0.170	0.187
ave. est.	$\hat{\Psi}_{rr}$	0.145	0.145	0.145	0.145	0.145
variance	$\hat{V}_t$	0.175	0.158	0.150	0.159	0.176
95% CI	$\hat{\Psi}_{rr}$	91.6	92.1	94.1	92.5	90.7
coverage	$\hat{V}_t$	94.0	93.4	94.6	93.7	93.6

Table 4.5. Chi-square(4) with n=25

	True value	0.4	1	4	8	12
	Empirical variance	0.241	0.233	0.213	0.253	0.442
ave. est.	$\hat{\Psi}_{rr}$	0.123	0.123	0.123	0.123	0.123
variance	$\hat{V}_t$	0.210	0.197	0.168	0.222	0.379
95% CI	$\hat{\Psi}_{rr}$	83.0	82.6	85.5	81.4	68.3
coverage	$\hat{V}_t$	92.4	91.5	90.5	92.9	91.9

Table 4.6. Chi-square(4) with n=50

	True value	0.4	1	4	8	12
	Empirical variance	0.205	0.200	0.164	0.229	0.320
ave. est.	$\hat{\Psi}_{rr}$	0.136	0.136	0.136	0.136	0.136
variance	$\hat{V}_t$	0.186	0.177	0.159	0.196	0.302
95% CI	$\hat{\Psi}_{rr}$	89.1	89.0	92.2	86.5	79.4
coverage	$\hat{V}_t$	92.9	93.2	94.8	93.1	92.6

Table 4.7. Chi-square(4) with n=100

	True value	0.4	1	4	8	12
	Empirical variance	0.177	0.174	0.165	0.166	0.245
ave. est.	$\hat{\Psi}_{rr}$	0.142	0.142	0.142	0.142	0.142
variance	$\hat{V}_t$	0.167	0.162	0.153	0.172	0.225
95% CI	$\hat{\Psi}_{rr}$	91.8	91.8	93.3	91.7	85.6
coverage	$\hat{V}_t$	94.0	93.6	94.0	95.7	93.3

Table 4.8. Chi-square(4) with n=200

	True value	0.4	1	4	8	12
	Empirical variance	0.161	0.159	0.149	0.150	0.180
ave. est.	$\hat{\Psi}_{rr}$	0.145	0.145	0.145	0.145	0.145
variance	$\hat{V}_t$	0.159	0.156	0.151	0.157	0.180
95% CI	$\hat{\Psi}_{rr}$	94.0	93.3	94.6	93.8	92.2
coverage	$\hat{V}_t$	94.9	94.1	95.1	95.0	95.5

Table 4.9. Uniform(2,8) with n=25

	True value	2.5	3.5	5	6.5	7.5
	Empirical variance	0.263	0.227	0.208	0.271	0.321
ave. est.	$\hat{\Psi}_{rr}$	0.122	0.122	0.122	0.122	0.122
variance	$\hat{V}_t$	0.220	0.182	0.173	0.226	0.297
95% CI	$\hat{\Psi}_{rr}$	81.5	83.9	85.8	80.0	76.3
coverage	$\hat{V}_t$	91.7	91.1	92.2	91.6	92.7

Table 4.10. Uniform(2,8) with n=50

	True value	2.5	3.5	5	6.5	7.5
	Empirical variance	0.234	0.191	0.174	0.174	0.203
ave. est.	$\hat{\Psi}_{rr}$	0.135	0.135	0.135	0.135	0.135
variance	$\hat{V}_t$	0.210	0.180	0.160	0.171	0.195
95% CI	$\hat{\Psi}_{rr}$	85.2	88.9	90.9	90.3	89.0
coverage	$\hat{V}_t$	93.8	93.5	93.6	94.5	94.7

Table 4.11. Uniform(2,8) with n=100

	True value	2.5	3.5	5	6.5	7.5
	Empirical variance	0.170	0.167	0.155	0.168	0.183
ave. est.	$\hat{\Psi}_{rr}$	0.142	0.142	0.142	0.142	0.142
variance	$\hat{V}_t$	0.174	0.162	0.154	0.160	0.173
95% CI	$\hat{\Psi}_{rr}$	93.8	92.2	93.8	91.9	91.3
coverage	$\hat{V}_t$	95.7	94.4	95.0	94.4	95.3

Table 4.12. Uniform(2,8) with n=200

	True value	2.5	3.5	5	6.5	7.5
	Empirical variance	0.157	0.162	0.162	0.155	0.155
ave. est.	$\hat{\Psi}_{rr}$	0.144	0.144	0.144	0.144	0.144
variance	$\hat{V}_t$	0.159	0.153	0.150	0.153	0.159
95% CI	$\hat{\Psi}_{rr}$	93.2	93.9	94.1	94.4	94.5
coverage	$\hat{V}_t$	94.3	94.6	94.5	95.3	95.7

Table 4.13. P-values for Normal distribution

Outlier cause:	κ_1	κ_2	κ_3
large f_t	0.02441	0.00536	0.37820
large v_t	0.00040	0.70990	0.00018
large f_t and v_t	0.00005	0.00043	0.00656

Table 4.14. P-values for Chi-square distribution

Outlier cause:	κ_1	κ_2	κ_3
large f_t	0.00690	0.00021	0.82924
large v_t	0.00049	0.42692	0.00025
large f_t and v_t	0.00020	0.00012	0.04613

5. Example

This section presents an application of our variance calculation to data from a substance abuse prevention study at the Institute for Social and Behavioral Research at Iowa State University. (See http://www.projectfamily.isbr.iastate.edu for project information.) The program was introduced to Iowa families with a child in the 6th grade. The measures of the study used in this example include self-reported levels of substance use, problem behaviors, and peer relations. The study followed these targets in a longitudinal study. We have taken 2 different time periods from this data, 8th grade and 10th grade measurements.

The latent construct used has gateway substance use (GSUI), alcohol use composite (AUCI), school-related problem behaviors (SRPB), conduct problems (DEBH), oppositional

hostility (OPAG), and affiliation with antisocial peers (AFPP) as six indicators for problem behaviors in children. These indicators are comprised of responses obtained from a self-report questionnaire. The substance use and alcohol use indexes are sums of yes/no responses for various substances, scored so that higher values represent a higher level of substance use. The other indicators cover a variety of problem behaviors related to skipping school, stealing, fighting, arguing, and similar issues regarding the behavior of their closest friends. These items are scaled on a five-point Likert-type scale and averaged for each indictor grouping. High scores of these measures indicate higher levels of problem behaviors. The alpha reliabilities for the items contained in each of the problem behavior scale measures for 8th grade measurements ranged between 0.55 and 0.83 and for 10th grade measurements ranged between 0.50 and 0.84.

We fit the measurement model

$$\begin{pmatrix} SRPB \\ AUCI \\ AFPP \\ OPAG \\ DEBH \\ GSUI \end{pmatrix} = \begin{pmatrix} 0 \\ \beta_{02} \\ \beta_{03} \\ \beta_{04} \\ \beta_{05} \\ \beta_{06} \end{pmatrix} + \begin{pmatrix} 1 \\ \beta_{12} \\ \beta_{13} \\ \beta_{14} \\ \beta_{15} \\ \beta_{16} \end{pmatrix} f_t + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{pmatrix}, \qquad t = 1,\ldots,100.$$

Using a portion of the data set, we randomly chose 100 students to illustrate the differences between using the variance $\hat{\Psi}_{rr}$ from (1.14) and the variance $\hat{V}_t$ from (3.1). We calculated the values of $\hat{f}_t$, $\hat{\Psi}_{rr}$ and $\hat{V}_t$ for the 8th grade and 10th grade measurements. At the 8th grade, we found $\hat{\Psi}_{rr}$=0.006 and the average of $\hat{V}_t$=0.011 with a minimum value of 0.009 and a maximum value of 0.028. At the 10th grade, we found $\hat{\Psi}_{rr}$=0.005 and the average value of

$\hat{V}_t$=0.012 with a minimum value of 0.010 and a maximum value of 0.020. This clearly shows that for every observation, the value of $\hat{\Psi}_{rr}$ was smaller than $\hat{V}_t$, which is shown in Figures 1 and 2. Note that $\hat{\Psi}_{rr}$ is labeled "standard variance" and $\hat{V}_t$ is labeled "higher order variance" in the legends of Figures 1 and 2.

Figure 1 shows the patterns for the variances in the 8th grade measurements. The variances $\hat{V}_t$ increase as the value of $\hat{f}_t$ increases. Figure 2 shows the variances for the 10th grade measurements. It shows less of a pattern for the $\hat{V}_t$ variances. These examples show that in some cases, not only are the $\hat{\Psi}_{rr}$ variances generally unbiased, but they may also miss possible trends in the true variances.

We also checked to see if we would get any indications of outliers in the data. Using our same formula for checking outliers, κ_2 (4.3), we compared results using κ_2 and then replacing $\hat{\Psi}_{rr}$ in place of $\hat{V}_t$ in κ_2. Using p-values with a Bonferroni adjustment to number of comparisons, we found using $\hat{\Psi}_{rr}$ indicated 6 outliers and using $\hat{V}_t$ indicated only 3 outliers for the 8th grade measurements. We also found that $\hat{\Psi}_{rr}$ indicated 17 outliers and $\hat{V}_t$ indicated only 1 outlier for the 10th grade measurements. Again we see that the bias in underestimation of the variance, $\hat{\Psi}_{rr}$, can considerably affect our analyses and conclusions. This example clearly demonstrates the usefulness of making the effort to correctly represent the variance of $\hat{f}_t$.

In conclusion, we have addressed true value estimation of latent variable constructs. We have provided an expression for the variance of factor score estimates that accounts for

the added measurement errors in inference. We have developed tools for inference regarding true values and diagnostics and directly shown the value of incorporating this adjustment into inference related to latent variables. Although we have not captured all of the variability in the variance of the factor score estimates, we have shown that in capturing the contribution of the estimation error that depends on the sample size and which gives correlation among factor score estimators for different individuals it is by far superior to current methods that ignore this added variability.

Figure 1: Variance Estimations 8th Grade

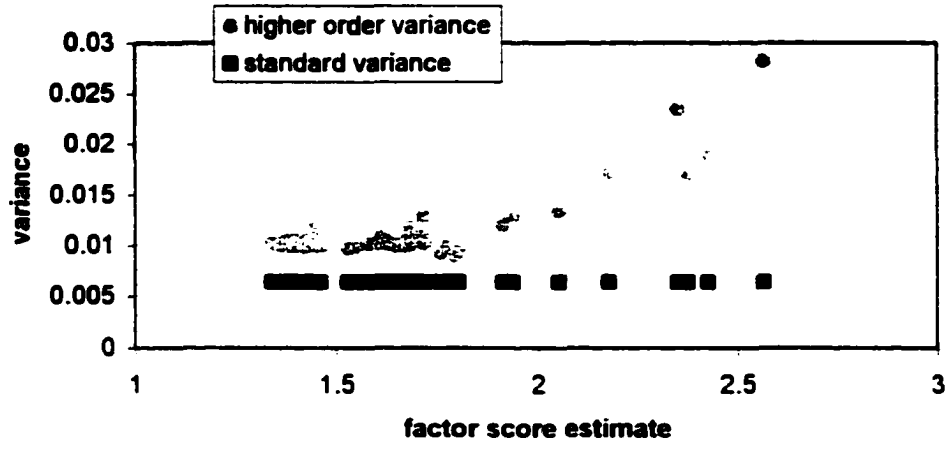
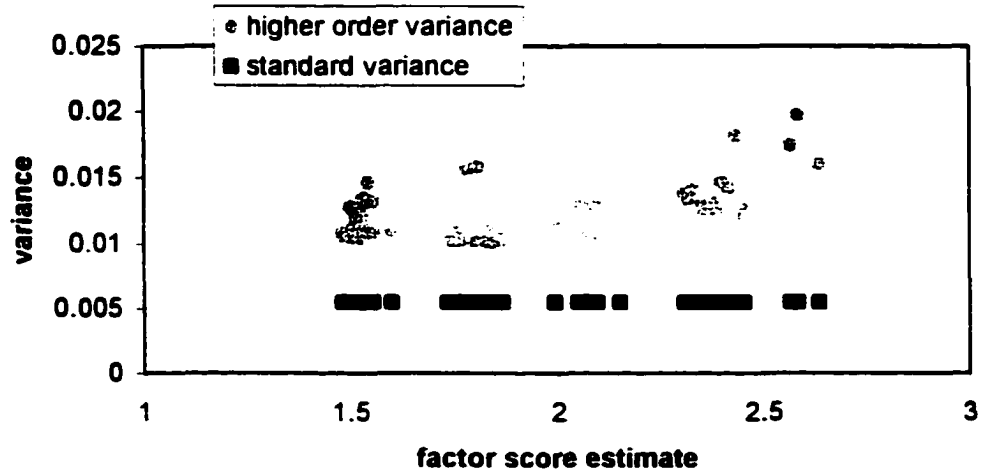


Figure 2: Variance Estimations 10th Grade



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GENERAL CONCLUSION

The goals of these papers were to present sound statistical methods for assessing intervention effects with a nonlinear relationship while incorporating covariate information and also to account for measurement errors in true value estimation of latent variable constructs. The extension from existing methods of linear models to incorporating nonlinearity in the intervention effects with covariate relationships is a gateway to further development of more sophisticated and statistically sound techniques. Our method gives verifiably consistent estimates of only the intervention effects, which usually are of main interest. There are many opportunities to expand and improve upon this and other currently available methods. Also, the presentation of a way to account for measurement error in true value estimation of latent variable constructs will likely lead to a wide variety of applications. The need for this improvement is well acknowledged and will hopefully be embraced by researchers.

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Computational complexity of digraph decomposition and the congruence extension property for algebras

by

Joy Lynne Becker

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ABSTRACT

The strong direct product is one of the standard graph products. In 1992, Feigenbaum and Schäffer presented a polynomial-time algorithm to find the unique prime factorization of connected graphs under the strong direct product. In this paper, we show that weakly connected directed graphs have unique prime factorizations with respect to the strong direct product, and we give a polynomial-time algorithm to find the prime factorizations of such digraphs. This is an extension of Feigenbaum and Schäffer's work on factoring undirected graphs under the strong direct product and Imrich's work on factoring undirected graphs with respect to the weak direct product.

We also investigate the problem of determining whether an algebra has the congruence extension property. We prove that this problem is complete for polynomial time.

CHAPTER 1. INTRODUCTION

Examining properties of graphs and algebraic structures oftens leads to questions about computational complexity. We can define a decision problem based on a property of an algebra or a class of algebras, with the goal of determining the complexity of the problem. In order for this to make sense, we assume our structures are finite. As an example, consider the following question: Given a finite algebra **A** of finite similarity type, does **A** have a proper subalgebra? In fact, this problem was shown to be complete for **P** by Bergman and Slutzki (2).

This area of computational complexity is of interest to algebraists because it gives them a sense of how hard it is to determine certain properties of algebras. It is also of interest to computer scientists because it gives them some natural mathematical examples of problems in the various complexity classes. This is especially true for some of the higher complexity classes, where there are not many examples available.

We consider two different problems in this paper. The first problem involves directed graphs. In graph theory, there are several different notions of graph products. Three of the standard ones are the Cartesian product, the weak direct product, and the strong direct product, which are formally defined in Chapter 2. Two fundamental questions arise from these notions of products: Given a graph, can it be represented as a nontrivial product of graphs, and how difficult is it to determine the factorization of a graph? For all three of these products, there are known polynomial-time algorithms to calculate the factorizations of connected graphs, with the added nonbipartite restriction for the weak product.

The definitions of graph products can be extended to directed graphs. In this paper we consider the complexity of factoring a weakly connected digraph with respect to the strong direct product. We present an algorithm to compute the prime factorization of a given di-

graph. In Theorem 3.7.3, we prove that the strong direct decomposition of such a digraph into prime factors is unique and that this decomposition can be found in polynomial time. Besides answering the existence question, our algorithm actually determines the unique factorization, if it exists.

The second problem we consider is based on the congruence extension property. An algebra $\mathbf{A}$ has the congruence extension property if any congruence on any subalgebra of $\mathbf{A}$ has an extension congruence on $\mathbf{A}$. For a formal definition, see Definition 4.0.1. For example, it can be shown that any Abelian group has the congruence extension property, but it is easy to find groups that do not have the congruence extension property. The group $\mathbf{A}_5$ of even permutations on five letters is one such group. We restrict the problem CEP to finite algebras of finite similarity type. Formally, it is defined as follows:

$$\text{CEP} = \{\mathbf{A} : \mathbf{A} \text{ has the congruence extension property}\}.$$

Given an algebra $\mathbf{A}$, the problem is to determine whether $\mathbf{A} \in \text{CEP}$. In Theorem 4.0.4, we prove that CEP is complete for polynomial time.

We begin with a summary of the relevant background material from graph theory, universal algebra, and complexity theory. Chapter 3 contains the results on digraph decomposition, and complexity of the congruence extension property problem is presented in Chapter 4. The final chapter includes a discussion of some related open problems.

CHAPTER 2. BACKGROUND

To understand the digraph decomposition and congruence extension property problems, we first need to define some concepts from graph theory, universal algebra, and complexity theory. We present only the definitions needed to understand the results in this paper. For further definitions and details, the reader should consult (5; 11) for graph theory, (4; 14) for universal algebra, and (15; 17) for complexity theory.

2.1 Graph Theory Preliminaries

We define a *graph* G as a set $V(G)$ of vertices together with an edge set $E(G)$ of unordered pairs $[x, y]$ of vertices of G. More precisely, this statement defines a *simple* graph G because the edge set contains no loops or multiple edges, where a *loop* is an edge $[x, x]$ from a vertex to the same vertex. A simple graph is *finite* if its vertex set is finite. A *directed graph* or *digraph* is a graph in which the edges have an orientation. The directed edge from x to y is denoted $x \to y$, and we say that y is *adjacent* to x. For a digraph G, the graph U with $V(U) = V(G)$ and edge set $E(U) = \{[x, y] : x \to y \in E(G) \text{ or } y \to x \in E(G)\}$ is called the *underlying graph* of G. In this paper, we mainly consider finite simple digraphs, but we state the following definitions for both graphs and digraphs.

A *subgraph* H of G is a graph H for which $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. If $[x, y] \in E(G)$ implies that $[x, y] \in E(H)$ for all pairs of vertices x and y of H, then H is called an *induced subgraph* of G. For H to be an *induced subdigraph*, we require that the edge orientation be preserved, so that $x \to y \in E(G)$ implies $x \to y \in E(H)$. We say a sub(di)graph H of G *spans* G if $V(H) = V(G)$.

Graphs G and H are *isomorphic*, denoted $G \cong H$, if there exists a bijection φ from $V(G)$

onto $V(H)$ such that $[x,y] \in E(G)$ if and only if $[\varphi(x), \varphi(y)] \in E(H)$. In the directed case, the orientation of edges must also be preserved by the mapping φ, so $G \cong H$ if $x \to y \in E(G)$ if and only if $\varphi(x) \to \varphi(y) \in E(H)$. Essentially, isomorphic (di)graphs are different (di)graphs with the same structure.

The *complete graph on n vertices*, denoted K_n, is the simple graph with all possible edges between vertices. In other words, for any two vertices $x \neq y$, there is an edge $[x,y]$. In the directed case, we define K_n to be the simple digraph for which $x \to y$ and $y \to x$ in K_n for any two vertices $x \neq y$.

A graph G is *connected* if for any two vertices x and y of G, there is a path from x to y. For a digraph G, if there is a directed path between any pair of vertices of G, then G is *connected*, and G is *weakly connected* if the underlying graph of G is connected. If a (di)graph is not connected, we say it is *disconnected*. In a disconnected (di)graph, the maximal connected sub(di)graphs are called *connected components*. The *weakly connected components* of a digraph are the connected components of its underlying graph.

The *open neighborhood* of a vertex x in a graph G, denoted $N_G(x)$ or simply $N(x)$, is the set of all vertices of G which are adjacent to x. So, $N(x) = \{y : [x,y] \in E(G)\}$. The *closed neighborhood* of x also includes the vertex x. We write $\overline{N}(x) = N(x) \cup \{x\}$. Note that if loops are allowed, it is possible to have $N(x) = \overline{N}(x)$. In the directed case, there is more than one definition for the neighborhood of a vertex because of the orientation of the edges. For our purposes, the open neighborhood of a vertex x in a digraph G is the set of all vertices which are adjacent to x. So, $N(x) = \{y : x \to y \in E(G)\}$. Note that this set does not include the vertices to which x is adjacent. The closed neighborhood of x is defined as above. If $\overline{N}(x) = \overline{N}(y)$, we call x and y *interchangeable* vertices. Note that in a simple digraph we have $\overline{N}(x) = \overline{N}(y)$ if and only if $x = y$ or $x \leftrightarrow y$ and for all z such that $z \neq x$ and $z \neq y$, $x \to z$ if and only if $y \to z$.

There are four standard types of graph products. We define three of them here. The first is the most fundamental type, the Cartesian product. The *Cartesian product* of two graphs G_1 and G_2 is denoted by $G_1 \Box G_2$ and defined by

$$V(G_1 \Box G_2) = V(G_1) \times V(G_2);$$

$$E(G_1 \square G_2) = \{[(x_1, x_2), (y_1, y_2)] : x_1 = y_1 \text{ and } [x_2, y_2] \in E(G_2) \text{ or}$$
$$[x_1, y_1] \in E(G_1) \text{ and } x_2 = y_2\}.$$

Note that in defining the vertex set, $\times$ represents the standard Cartesian product of sets. The Cartesian product is commutative and associative and has the trivial simple graph K_1 as a unit. The Cartesian product of two graphs is connected if and only if both factors are connected (11).

Figure 2.1 shows the Cartesian product of the complete graphs K_2 and K_3. Note that there are three distinct copies of K_2 and two distinct copies of K_3 in the product graph.

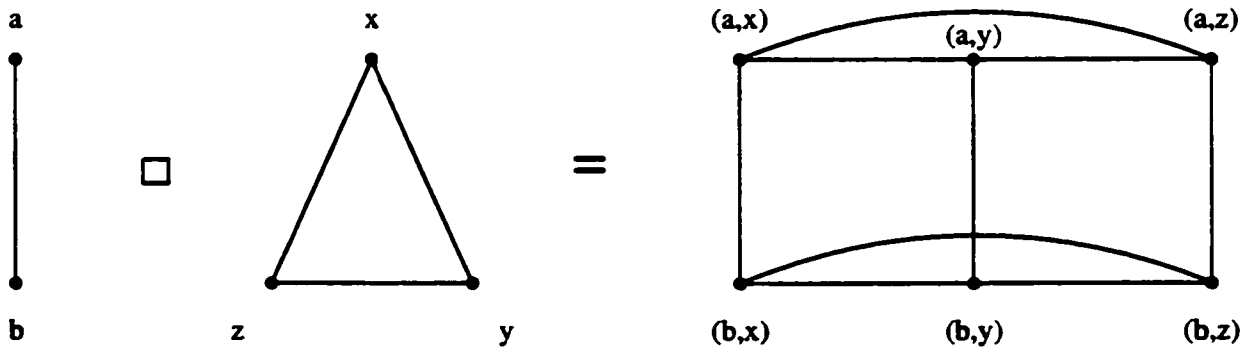

Figure 2.1 The Cartesian product $K_2 \square K_3$

The *weak direct product* or *cardinal product* of G_1 and G_2, denoted $G_1 \times G_2$, is defined by

$$V(G_1 \times G_2) = V(G_1) \times V(G_2);$$

$$E(G_1 \times G_2) = \{[(x_1, x_2), (y_1, y_2)] : [x_1, y_1] \in E(G_1) \text{ and } [x_2, y_2] \in E(G_2)\}.$$

The weak direct product is also commutative and associative. In the class of simple graphs it has no unit, but if loops are allowed, the one vertex graph with a loop is a unit. It is possible for the weak direct product of two graphs to be disconnected even if both factors are connected. For example, the product $K_2 \times K_2$ is disconnected. However, it has been shown that the weak

direct product of two graphs is connected if and only if both factors are connected and at least one of the factors is nonbipartite (10).

Figure 2.2 shows the weak direct product of the complete graphs K_2 and K_3. Note that the product graph is isomorphic to the cycle of length six.

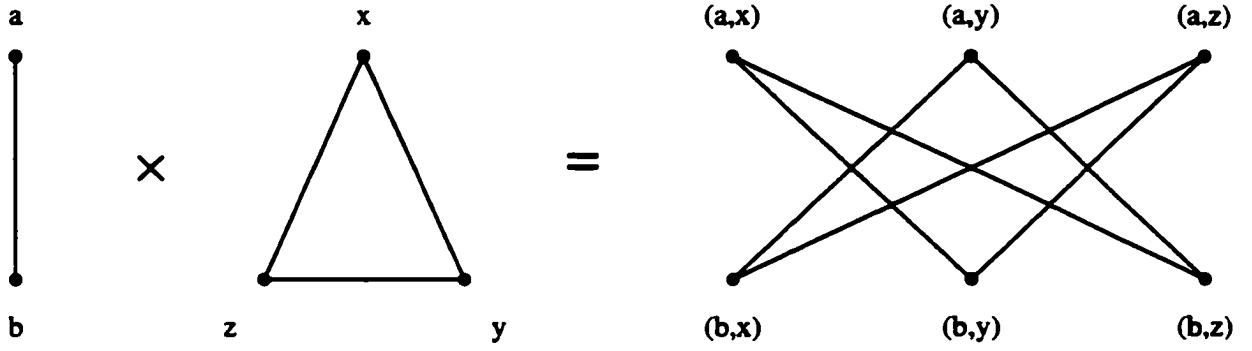

Figure 2.2 The weak direct product $K_2 \times K_3$

The *strong direct product*, or simply the *strong product*, of G_1 and G_2 is denoted by $G_1 \boxtimes G_2$ and defined by

$$V(G_1 \boxtimes G_2) = V(G_1) \times V(G_2);$$

$$\begin{aligned} E(G_1 \boxtimes G_2) = \{[x_1, x_2], [y_1, y_2] : {} & x_1 = y_1 \text{ and } [x_2, y_2] \in E(G_2) \text{ or} \\ & [x_1, y_1] \in E(G_1) \text{ and } x_2 = y_2 \text{ or} \\ & [x_1, y_1] \in E(G_1) \text{ and } [x_2, y_2] \in E(G_2)\}. \end{aligned}$$

We could also write $E(G_1 \boxtimes G_2) = E(G_1 \square G_2) \cup E(G_1 \times G_2)$. The strong product is commutative and associative with K_1 as a unit. The strong product of two graphs is connected if and only if both factors are connected (9). The notation for these three products comes from the product of an edge with itself and was introduced by Nešetřil.

Figure 2.3 shows the strong product of the complete graphs K_2 and K_3. Note that the edge set is the union of the edges from the corresponding Cartesian and weak direct products.

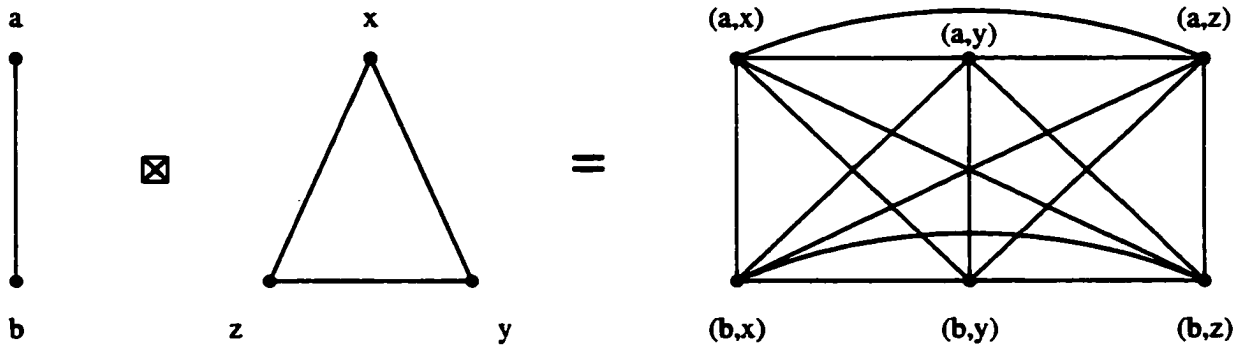

Figure 2.3 The strong product $K_2 \boxtimes K_3$

All three of these product definitions can be extended to digraphs, and we use the same notation. The vertex sets remain the same, with the edge sets defined in the following manner:

$$E(G_1 \square G_2) = \{(x_1, x_2) \to (y_1, y_2) : x_1 = y_1 \text{ and } x_2 \to y_2 \in E(G_2) \text{ or } x_1 \to y_1 \in E(G_1) \text{ and } x_2 = y_2\};$$

$$E(G_1 \times G_2) = \{(x_1, x_2) \to (y_1, y_2) : x_1 \to y_1 \in E(G_1) \text{ and } x_2 \to y_2 \in E(G_2)\};$$

$$E(G_1 \boxtimes G_2) = E(G_1 \square G_2) \cup E(G_1 \times G_2).$$

The products remain commutative and associative, and the Cartesian and strong products have K_1 as a unit. If loops are allowed, the weak direct product has the one vertex graph with a loop as a unit.

Figures 2.4, 2.5, and 2.6 show the three products of the directed edge D with the directed triangle T, where $E(D) = \{a \to b\}$ and $E(T) = \{x \to y, y \to z, z \to x\}$. The Cartesian product digraph has the Cartesian product graph $K_2 \square K_3$ as its underlying graph. The weak direct product digraph is quite different from the undirected product, and it is isomorphic to the digraph with three disconnected directed edges. The strong product edge set is again the union of the Cartesian and weak directed edges from the other two product graphs.

A *prime* or *irreducible* (di)graph is one that cannot be expressed as the product of two

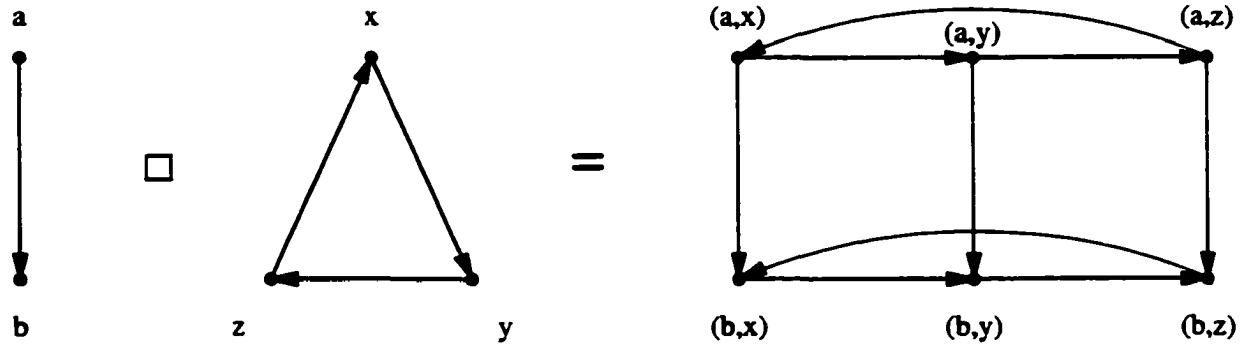

Figure 2.4 The Cartesian product $D \square T$

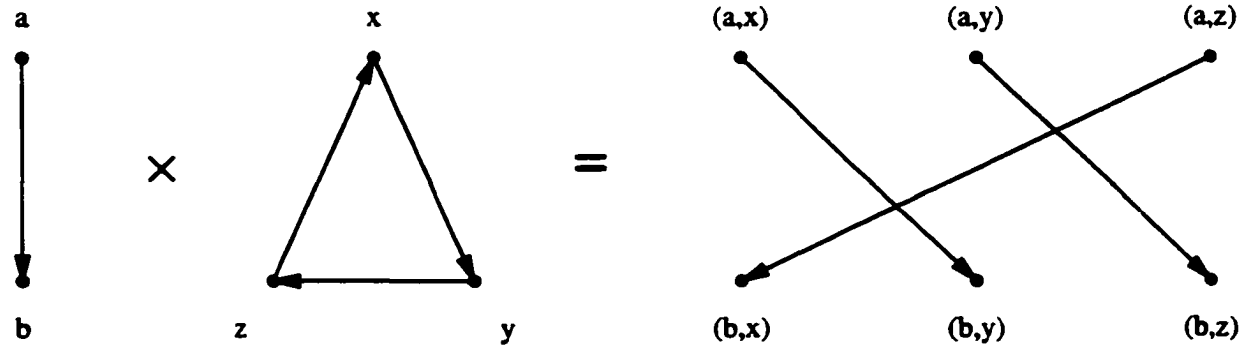

Figure 2.5 The weak direct product $D \times T$

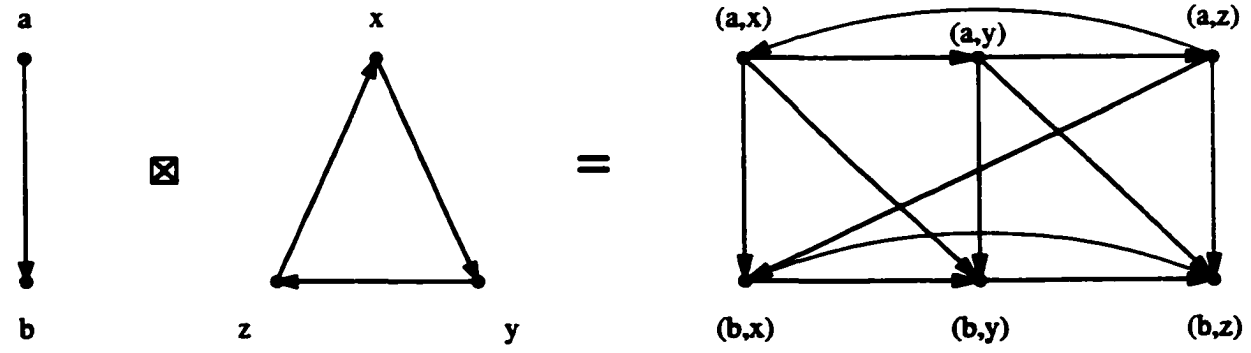

Figure 2.6 The strong product $D \boxtimes T$

nontrivial (di)graphs. Note that this definition of primality depends on the product type. For example, there exist (di)graphs which are irreducible with respect to the strong product but factorable under the Cartesian product. The cycle of length four is one such graph. It is true that most graphs are prime (9). Note that the complete (di)graph K_p, where p is a prime, is irreducible with respect to all three products. We are interested in knowing which product operators have the *unique prime factorization property*, which says that for every (di)graph G, there is a unique set of prime (di)graphs $G_1, G_2, \ldots, G_k$ such that G is the product of the G_i's and $G_i \neq K_1$ for all $1 \leq i \leq k$. Such a factorization is called a *unique prime factor decomposition* or a UPFD of the (di)graph G.

In this paper, we are mainly interested in the strong product of digraphs, so we introduce a few more definitions related to this product. Suppose a digraph G has been factored into k prime factors, $G = G_1 \boxtimes G_2 \boxtimes \cdots \boxtimes G_k$. Then each vertex x has a coordinatization $(x_1, x_2, \ldots, x_k)$. The number of coordinates of a vertex and the number of coordinates in which two vertices differ are independent of the representation of G, so every vertex on G has a *unique coordinatization.* We say that each factor G_i *divides* G or that G is *divisible* by G_i with respect to the strong product. To emphasize the dependence of divisibility on the type of product, we use $\boxtimes$-divisible to denote divisibility with respect to the strong product. An edge of G is called a *Cartesian edge* if the coordinates of its endpoints differ in exactly one component. Otherwise, it is called a *weak direct edge.* The *ith projection map* $p_i : G \to G_i$ is defined by $p_i(x_1, x_2, \ldots, x_k) = x_i$. The subdigraph induced by all vertices with coordinates $(x_1, \ldots, x_{i-1}, \cdot, x_{i+1}, \ldots, x_k)$, where the ith component ranges over all vertices of G_i, is called a *copy* of G_i. We denote by G_i^a the G_i-copy induced by the set $\{x \in V(G) : x_j = a_j \text{ for all } j \neq i\}$, where $a = (a_1, \ldots, a_k)$. We could also write $G_i^a = \{x \in V(G) : p_j(x) = a_j \text{ for } j \neq i\}$. This definition of a copy of a factor also holds for the Cartesian and weak direct products. The closed neighborhood of a vertex x in G can be expressed as $\overline{N}_G(x) = \overline{N}_{G_1}(x_1) \times \overline{N}_{G_2}(x_2) \times \cdots \overline{N}_{G_k}(x_k)$. We will write $\overline{N}_i$ for $\overline{N}_{G_i}$.

2.2 Universal Algebra Preliminaries

For a set A and a nonnegative integer n, A^n denotes the set of n-tuples of elements of A. An *n-ary operation* on A is a function $f : A^n \to A$. The integer n is called the *rank* or *arity* of f. If an operation f on A has rank 0, then f is called a *nullary* or *constant* operation. Because a nullary operation is determined by the value $f(\emptyset) \in A$, it is often thought of as an element of A.

An *algebra* is an ordered pair $\mathbf{A} = \langle A, F \rangle$, where A is a nonempty set and F is a set of operations on A. The set A is called the *universe* of $\mathbf{A}$, and F is the set of *basic* or *fundamental operations* of $\mathbf{A}$. An algebra $\mathbf{A}$ is *finite* if $|A|$ is finite, and $\mathbf{A}$ is *trivial* if $|A| = 1$. If F is finite, then we say $\mathbf{A}$ is of *finite similarity type*. If $\mathbf{A} = \langle A, F \rangle$ and $\mathbf{B} = \langle A, G \rangle$ with $G \subseteq F$, then we call the algebra $\mathbf{B}$ a *reduct* of $\mathbf{A}$, and the algebra $\mathbf{A}$ is called an *expansion* of $\mathbf{B}$.

A set B is a *subuniverse* of the algebra $\mathbf{A}$ if $B \subseteq A$ and if B is closed under the basic operations of $\mathbf{A}$. In particular, the *subuniverse of $\mathbf{A}$ generated by X*, denoted $\mathrm{Sg}^{\mathbf{A}}(X)$, is the smallest subuniverse of $\mathbf{A}$ which contains X. To be precise,

$$\mathrm{Sg}^{\mathbf{A}}(X) = \bigcap \{B : X \subseteq B \text{ and } B \text{ is a subuniverse of } \mathbf{A}\}.$$

If X is empty, then $\mathrm{Sg}^{\mathbf{A}}(\emptyset) = \{c : \text{c is a constant operation of } \mathbf{A}\}$. Note that if $\mathbf{A}$ has no constant operations, then $\mathrm{Sg}^{\mathbf{A}}(\emptyset) = \emptyset$. $\mathbf{B} = \langle B, G \rangle$ is a *subalgebra* of $\mathbf{A}$, denoted $\mathbf{B} \leq \mathbf{A}$, if B is a subuniverse of $\mathbf{A}$ and the operations in G are the operations of F restricted to elements of B. We write $G = F \restriction_B$. The empty set may be a subuniverse of $\mathbf{A}$, but it is never the universe of a subalgebra of $\mathbf{A}$.

Let θ be an equivalence relation on A. We define θ to be a *congruence* on $\mathbf{A}$ if for all $f \in F$ and for all pairs $(a_i, b_i) \in \theta, i = 1, \ldots, n$,

$$(f(a_1, \ldots a_n), f(b_1, \ldots b_n)) \in \theta,$$

where n is the rank of f. In general, if the above condition holds for an operation f, we say *f preserves θ*. If every f in F preserves θ, then we say the set F preserves θ. The set of all congruences of an algebra $\mathbf{A}$ is denoted $\mathrm{Con}(\mathbf{A})$. The smallest element of $\mathrm{Con}(\mathbf{A})$ is the identity

relation $\delta_A = \{(x,x) : x \in A\}$, and the largest element is the relation $A^2 = \{(x,y) : x,y \in A\}$. For $\nu \subseteq A \times A$, the *congruence on* $\mathbf{A}$ *generated by* ν, denoted $\mathrm{Cg}^{\mathbf{A}}(\nu)$, is the smallest congruence on $\mathbf{A}$ which contains ν. To be precise,

$$\mathrm{Cg}^{\mathbf{A}}(\nu) = \bigcap \{\theta \in \mathrm{Con}(\mathbf{A}) : \nu \subseteq \theta\}.$$

In particular, $\mathrm{Cg}^{\mathbf{A}}(a,b) = \bigcap \{\theta \in \mathrm{Con}(\mathbf{A}) : (a,b) \in \theta\}$. If a congruence θ can be generated by a single pair of elements, then θ is called a *principal congruence.* A nontrivial algebra $\mathbf{A}$ is said to be *simple* if $\mathrm{Con}(\mathbf{A}) = \{\delta_A, A^2\}$.

2.3 Complexity Theory Preliminaries

Most problems in computational complexity are defined in terms of languages, where a *language* is a set of finite strings over a fixed alphabet. For each language L, we can define a decision problem: Given a string x, is x in L? The amount of time or space required to answer this question generally depends on the length of the input string x. If there is a polynomial p such that some deterministic Turing machine can decide whether an input string x of length n lies in a language L in time $O(p(n))$, then we say L is computable in *polynomial time.* Let $\mathbf{P}$ denote the set of all languages computable in polynomial time.

We say L is computable in *nondeterministic log-space* if there is a nondeterministic Turing machine which can decide whether x lies in L in space $O(\log n)$. The set of all languages which are computable in nondeterministic log-space is denoted **NL**. If L can be decided by a nondeterministic Turing machine in polynomial time, then we say L is computable in *nondeterministic polynomial time.* Let **NP** denote the set of all such languages. **NP** can also be defined as the class of languages for which a solution can be verified in polynomial time. It can be shown that $\mathbf{NL} \subseteq \mathbf{P} \subseteq \mathbf{NP}$ (17). Although still unproven, it is believed that both of these inclusions are proper.

Given two problems A and B, we say that A is *log-space reducible* to B if there is a function f, which is computable in deterministic log-space, such that for every instance x of A, $x \in$ A if and only if $f(x) \in$ B. We denote this by A $\leq_{\log}$ B. If every member of **P** is log-space reducible

to B, then B is said to be *hard for* **P**. B is *complete for* **P** or **P**-*complete* if B is in **P** and is hard for **P**. Note that the relation $\leq_{\log}$ is reflexive and transitive. It follows that if A is **P**-complete, A $\leq_{\log}$ B, and B is in **P**, then B is **P**-complete. Also note that a problem A which is complete for **P** is at least as hard as every other problem in **P**. Thus, since **NL** $\subseteq$ **P** and the inclusion is believed to be proper, it is unlikely that a **P**-complete problem A belongs to the class **NL**.

We would like to state our problems in terms of mathematical properties rather that formal languages. To do this, we need to assume some reasonable encoding of the instances of a problem into finite strings. All graphs and digraphs are assumed to be simple and finite. The vertices of a (di)graph can be assumed to be $\{0, 1, \ldots, n-1\}$, and the edges can be represented by an adjacency matrix with indices $\{0, 1, \ldots, n-1\}$ and entries from $\{0, 1\}$. Thus, an input instance to the digraph decomposition problem has size at least n^2.

Similarly, we assume all algebras are finite and of finite similarity type. We can take the universe of an algebra to be $\{0, 1, \ldots, n-1\}$. This set can be represented in the input by its cardinality, which requires $\log n$ bits of storage. Each operation can be represented by a table of values. A k-ary operation will be represented as a k-dimensional array, with indices and entries coming from $\{0, 1, \ldots, n-1\}$. Such an array takes space $n^k \cdot \log n$ bits. Suppose $\mathbf{A} = \langle A, F \rangle$ is an algebra with $|A| = n$ and $|F| = q$, and suppose that the maximum rank of any operation in F is r. Then as an input instance to CEP, the size of $\mathbf{A}$ is at least $\max(n^r, nq)$.

Following the conventions of Imrich (11), we use the random-access machine as our model of computation. We also take the running time of an algorithm to be equivalent to the number of steps in its execution.

CHAPTER 3. DIGRAPH DECOMPOSITION

In this chapter we show that the prime factorization of weakly connected digraphs with respect to the strong product can be found in polynomial time. We also show that this factorization is unique. The general idea is to construct a Cartesian subdigraph which has a decomposition that is compatible with any strong decomposition of the original digraph. This Cartesian subdigraph can be factored under the Cartesian product using Feigenbaum's algorithm (8), and the factorization of the original digraph can be retrieved from this Cartesian decomposition. Unless stated otherwise, all digraphs in this chapter are assumed to be finite and simple. We begin with a discussion of some previous results regarding the complexity of graph decompositions.

3.1 Previous Results

There are many known results for decompositions of undirected graphs under the Cartesian, weak direct, and strong products. In 1960, Sabidussi showed that finite connected simple graphs have unique prime factor decompositions under the Cartesian product (16). This was perhaps the main introduction to the theory of graph multiplication. It was proven that connected simple graphs have unique prime factorizations under the strong product by Dörfler and Imrich in 1970 (7), and independently, by McKenzie in 1971 (13). McKenzie's work actually showed that nonbipartite connected graphs have unique factorizations with repsect to the weak direct product in the class of undirected graphs with loops. By the definitions of the weak direct direct and strong products, this implies the uniqueness result for the strong product.

Following the uniqueness results, the problem was to actually determine these prime fac-

tors. In particular, the complexity of these prime factorization problems was of interest. For the Cartesian product, Feigenbaum, Herschberger, and Schäffer presented a polynomial-time algorithm to find the unique factorization of connected simple graphs in 1985 (9). Their result utilized the towers of equivalence relations introduced by Sabidussi. Independently, Winkler presented a different polynomial-time algorithm in 1987, in which he regarded graphs as metric spaces (18). Their work inspired faster algorithms to be developed, and in 1992, Aurenhammer, Hagauer, and Imrich presented an algorithm which runs in $O(m \log n)$ time, where m is the number of edges of the graph and n is the number of vertices (1). This is currently the fastest known algorithm for factoring graphs with respect to the Cartesian product.

Similar results were found for the strong and weak direct factorizations of graphs. In 1992, Feigenbaum and Schäffer proved that connected simple graphs can be factored with respect to the strong product in polynomial time (9). For the weak direct product, Imrich presented a polynomial-time algorithm to find the factorization of nonbipartite connected graphs in the class of undirected graphs with loops in 1998 (10).

Although there are many known results for the complexity of graph decompositions, not much has been done with the factorization of directed graphs. In 1986, Feigenbaum extended the Cartesian factorization results to the directed graph case, showing that weakly connected digraphs have unique prime factorizations that can be determined in polynomial time (8). This work utilized the Cartesian factorization of undirected graphs. For the other two products, no results have been published. The methods of this chapter closely follow the work done by Feigenbaum and Schäffer in factoring graphs with respect to the strong product (9) and Imrich's work in factoring graphs under the weak direct product (10).

3.2 The Relation S and S-thin Digraphs

Define a relation S on the vertex set of a digraph G as follows: For vertices u and v in $V(G)$, uSv if and only if $\overline{N}(u) = \overline{N}(v)$. It is straightforward to check that S is an equivalence relation. Now define the digraph G/S as follows:

$$V(G/S) = \{D_i : D_i \text{ is an equivalence class of } S\};$$

$$E(G/S) = \{D_i \to D_j : i \neq j \text{ and there exist } u \in V(D_i) \text{ and } v \in V(D_j)$$
$$\text{such that } u \to v \in E(G)\}.$$

A digraph G is said to be *S-thin* if $S = \delta_G = \{(x,x) : x \in V(G)\}$. Clearly, G/S is S-thin. Note also that G is S-thin if and only if G has no interchangeable vertices. It can also be shown that if $G = G_1 \boxtimes G_2$, then G is S-thin if and only if G_1 and G_2 are S-thin.

Lemma 3.2.1. *Let G be a digraph with n vertices and m edges. Then G/S can be constructed in $O(n^3)$ time.*

Proof. Let $\{a,b\}$ be any pair of vertices in G. To check whether aSb, it suffices to check if $a \to x$ and $b \to x$ for all $x \in V(G)$. There are a total of n^2 pairs $\{a,b\}$ of vertices in G, and the adjacencies for each vertex can be checked in $O(n)$ time. Thus, the total time to determine which pairs of vertices are equivalent under S is $O(n^3)$.

Constructing the equivalence classes of S is equivalent to finding the weakly connected components of the digraph G', where $V(G') = V(G)$ and $a \to b$ in G' if aSb. The complexity of finding weakly connected components of a digraph is bounded by the number of edges, so the equivalence classes can be found in $O(n^2)$ time.

Finally, to construct the digraph G/S, the adjacencies of the equivalence classes need to be checked. This amounts to checking edges, which can be done in $O(m) < O(n^2)$ time. Therefore, G/S can be constructed in $O(n^3)$ time. □

3.3 Complete Factors

The first step in decomposing a digraph into prime factors is to determine the largest complete factor. For our problem, a complete digraph is defined as a graph with all possible directed edges, so a digraph G is complete if for any pair of vertices, $x \neq y$ in $V(G)$, $x \leftrightarrow y \in E(G)$. To factor out the largest complete digraph with respect to the strong product, we follow the direction of Imrich in finding the largest complete graph factor with respect to the weak direct product (10).

Lemma 3.3.1. $V((G \boxtimes H)/S) = \{U \times W : U \in V(G/S) \text{ and } W \in V(H/S)\}$.

Proof. Let $U \in V(G/S)$ and $W \in V(H/S)$. First we show that the vertices in $U \times W$ belong to the same equivalence class of $V((G \boxtimes H)/S)$. Let $(u_1, w_1), (u_2, w_2) \in U \times W$. Since U and W are equivalence classes of G/S and H/S, respectively, we have $u_1 S u_2$ and $w_1 S w_2$. Then $u_1 = u_2$ or $u_1 \leftrightarrow u_2 \in E(G)$ and $w_1 = w_2$ or $w_1 \leftrightarrow w_2 \in E(H)$. If $(u_1, w_1) = (u_2, w_2)$, then clearly $(u_1, w_1) S (u_2, w_2)$. If not, then by the definition of the strong product, $(u_1, w_1) \leftrightarrow (u_2, w_2) \in E(G \boxtimes H)$. It remains to be shown that for all $(x, y) \in G \times H$, with $(x, y) \neq (u_1, w_1)$ and $(x, y) \neq (u_2, w_2)$, $(u_1, w_1) \rightarrow (x, y)$ if and only if $(u_2, w_2) \rightarrow (x, y)$.

Let $(x, y) \in G \times H$ with $(x, y) \neq (u_1, w_1)$ and $(x, y) \neq (u_2, w_2)$, and suppose $(u_1, w_1) \rightarrow (x, y)$. By the definition of the strong product, we have the following cases:

Case 1. $u_1 = u_2, w_1 \leftrightarrow w_2$:

Note that since $w_1 S w_2$, $w_1 \rightarrow y \in E(H)$ if and only if $w_2 \rightarrow y \in E(H)$.

i. If $u_1 = x$ and $w_1 \rightarrow y$, then $u_2 = x$ and $w_2 \rightarrow y$.

ii. If $u_1 \rightarrow x$ and $w_1 = y$, then $u_2 \rightarrow x$ and $w_2 \rightarrow y$.

iii. If $u_1 \rightarrow x$ and $w_1 \rightarrow y$, then $u_2 \rightarrow x$ and $w_2 \rightarrow y$.

Case 2. $u_1 \leftrightarrow u_2, w_1 = w_2$:

Note that since $u_1 S u_2$, $u_1 \rightarrow x \in E(G)$ if and only if $u_2 \rightarrow x \in E(G)$.

i. If $u_1 = x$ and $w_1 \rightarrow y$, then $u_2 \rightarrow x$ and $w_2 \rightarrow y$.

ii. If $u_1 \rightarrow x$ and $w_1 = y$, then $u_2 \rightarrow x$ and $w_2 = y$.

iii. If $u_1 \rightarrow x$ and $w_1 \rightarrow y$, then $u_2 \rightarrow x$ and $w_2 \rightarrow y$.

Case 3. $u_1 \leftrightarrow u_2, w_1 \leftrightarrow w_2$:

i. If $u_1 = x$ and $w_1 \rightarrow y$, then $u_2 \rightarrow x$ and $w_2 \rightarrow y$.

ii. If $u_1 \rightarrow x$ and $w_1 = y$, then $u_2 \rightarrow x$ and $w_2 \rightarrow y$.

iii. If $u_1 \rightarrow x$ and $w_1 \rightarrow y$, then $u_2 \rightarrow x$ and $w_2 \rightarrow y$.

In all of the above cases, it follows that $(u_2, w_2) \rightarrow (x, y)$ by the definition of the strong product. We have shown that if $(u_1, w_1) \rightarrow (x, y)$, then $(u_2, w_2) \rightarrow (x, y)$. By a symmetric argument the converse holds, so $(u_1, w_1) S (u_2, w_2)$.

It remains to be shown that $U \times W$ is by itself an equivalence class of $(G \boxtimes H)/S$. Let $(u, w) \in U \times W$, and suppose that $(a, b) \neq (u, w)$ belongs to the same equivalence class as the vertices in $U \times W$. We need to show that $(a, b) \in U \times W$. Note that since $(a, b)S(u, w)$, for every $(x, y) \in U \times W$ with $(x, y) \neq (a, b)$ and $(x, y) \neq (u, w)$, we have $(a, b) \to (x, y)$ if and only if $(u, w) \to (x, y)$. Also, since $(a, b) \neq (u, w)$ and $(a, b)S(u, w)$, we have $(a, b) \leftrightarrow (u, w) \in E(G \boxtimes H)$. Consider the following cases:

Case 1. $a = u$ and $b \leftrightarrow w$:

Let $y \in V(H)$ with $y \neq b$ and $y \neq w$. Then

$$\begin{aligned} w \to y \in E(H) &\Leftrightarrow (u, w) \to (u, y) \in E(G \boxtimes H) \\ &\Leftrightarrow (a, b) \to (u, y) \in E(G \boxtimes H) \\ &\Leftrightarrow b \to y \in E(H), \text{ since } b \neq y. \end{aligned}$$

So bSw, and thus, $b \in W$.

Case 2. $a \leftrightarrow u$ and $b = w$:

Let $x \in V(G)$ with $x \neq a$ and $x \neq u$. Then

$$\begin{aligned} u \to x \in E(G) &\Leftrightarrow (u, w) \to (x, w) \in E(G \boxtimes H) \\ &\Leftrightarrow (a, b) \to (x, w) \in E(G \boxtimes H) \\ &\Leftrightarrow a \to x \in E(G), \text{ since } a \neq x. \end{aligned}$$

So aSu, and thus, $a \in U$.

Case 3. $a \leftrightarrow u$ and $b \leftrightarrow w$:

Let $x \in V(G)$ with $x \neq a$ and $x \neq u$. Then

$$\begin{aligned} u \to x \in E(G) &\Leftrightarrow (u, w) \to (x, w) \in E(G \boxtimes H), \\ &\Leftrightarrow (a, b) \to (x, w) \in E(G \boxtimes H) \\ &\Leftrightarrow a \to x \in E(G), \text{ since } a \neq x. \end{aligned}$$

So, aSu. By a symmetric argument we have bSw, and thus, $(a, b) \in U \times W$.

Therefore, $U \times W$ is an equivalence class of S. □

Proposition 3.3.2. *Let G and H be digraphs. Then $(G \boxtimes H)/S \cong G/S \boxtimes H/S$.*

Proof. This statement follows from Lemma 3.3.1 and the definition of the strong product. □

Lemma 3.3.3. *Let G be a weakly connected digraph and let $k > 1$ divide $|D_i|$ for all $D_i \in V(G/S)$. Then there exists a digraph H such that $G \cong K_k \boxtimes H$. Conversely, if $G \cong K_k \boxtimes H$ for some $k > 1$, then k divides $|D_i|$ for all $D_i \in V(G/S)$.*

Proof. Let $V(G/S) = \{D_i : i \in I\}$, and let $\{D_i' : i \in I\}$ be a family of disjoint sets with $|D_i| = k|D_i'|$. Define a digraph H as follows:

$$V(H) = \bigcup_{i \in I} D_i';$$

$$E(H) = \{x \to y : x, y \in V(D_i') \text{ or } x \in V(D_i'), y \in V(D_j'), \text{ and } D_i \to D_j \in E(G/S)\}.$$

Then $G \cong K_k \boxtimes H$.

For the converse, suppose that $G \cong K_k \boxtimes H$ for some $k > 1$. Since $V(K_k)$ is the only equivalence class of K_k/S, Lemma 3.3.1 implies that $V(G/S) = \{V(K_k) \times W : W \in V(H/S)\}$. Then it is clear that k divides $|D_i|$ for any $D_i \in V(G/S)$. □

Lemma 3.3.4. *Let $G \cong K_k \boxtimes H$ and $G \cong K_k \boxtimes H'$. Then $H \cong H'$.*

Proof. If $G = K_k \boxtimes H$, then $G/S \cong K_k/S \boxtimes H/S \cong H/S$ by Proposition 3.3.2, since K_k/S is the unit digraph K_1. Similarly, $G/S \cong H'/S$. So there is an isomorphism $\pi : H/S \cong H'/S$. This isomorphism can be chosen so that $|D_i| = |\pi(D_i)|$ for all $D_i \in V(H/S)$. Let $\varphi_i : D_i \to \pi(D_i)$ be a bijection. Then $\varphi : V(H) \to V(H')$ defined by $\varphi \restriction_{D_i} = \varphi_i$ gives an isomorphism $H \cong H'$. □

Lemma 3.3.5. *Let G be a weakly connected digraph with decompositions $G = K_m \boxtimes H$ and $G = K_n \boxtimes H'$. If H and H' are not $\boxtimes$-divisible by K_k for any $k > 1$, then $m = n$ and $H \cong H'$.*

Proof. Let $d = \gcd(\{|D_i| : D_i \in V(G/S)\})$. By Lemma 3.3.3, m divides d. Then $\{\frac{1}{m}|D_i|\}$ represents the size of the equivalence classes of H/S. The greatest common divisor of $\{\frac{1}{m}|D_i|\}$ must be 1, since H is not divisible by K_k for any $k > 1$. Therefore, $m = d$. By a symmetric argument, $n = d$, so $m = n$. Then by Lemma 3.3.4, $H \cong H'$. □

By Lemma 3.3.3, the largest complete factor of G can be determined by calculating the largest integer k such that k divides $|D_i|$ for all $D_i \in V(G/S)$. Since S and G/S can be constructed in polynomial time and the greatest common divisor of $\{|D_i| : D_i \in V(G/S)\}$ can be found in polynomial time using the Euclidean algorithm (5), the largest complete factor of G can also be determined in polynomial time. By Lemma 3.3.5, once the largest complete digraph is factored out of G, the remaining factor is uniquely determined.

3.4 Cartesian Edges and the Copy Consistency Property

Recall that an edge $(x_1, x_2) \to (y_1, y_2)$ is *Cartesian* with respect to the decomposition $G_1 \boxtimes G_2$ if either $x_1 = y_1$ or $x_2 = y_2$. A set of edges satisfies the *copy consistency property* if for every factor G_i, $i = 1, 2$, and every pair of adjacent vertices $x_i \to y_i \in V(G_i)$, the (copy of the) edge $x_i \to y_i$ is marked in all copies of the factor G_i or in no copies of G_i. By associativity of the strong product, the copy consistency property extends to any finite number of factors of G. The lemmata in this section are the basis for the algorithm presented in Section 3.5. The goal is to mark enough Cartesian edges to span G while satisfying the copy consistency property.

Lemma 3.4.1. *Let G be a weakly connected, nontrivial, S-thin digraph with $G = G_1 \boxtimes G_2$. Let F be a copy consistent set of directed Cartesian edges of G, and let H be the digraph with $V(H) = V(G)$ and $E(H) = F$.*

For all $x \in V(G)$, let

$$S(x) = \{y \in V(G) : \overline{N}(y) \subset \overline{N}(x)\},$$

$$P(x) = \{z \in V(G) : z \text{ is in the weakly connected component of } H \text{ which contains } x\},$$

$$R(x) = V(H) \setminus P(x), \text{ and}$$

$$\mathcal{J}(x) = \{\overline{N}(y) : y \in R(x) \cap S(x)\}.$$

Mark $x \to y$ if $\overline{N}(y)$ is maximal in $\mathcal{J}(x)$. Then all marked edges are Cartesian and the set of all marked edges satisfies the copy consistency property.

Proof. We begin by showing that every marked edge is Cartesian. Let $x = (x_1, x_2)$ and $y = (y_1, y_2)$. Suppose $x \to y$ is marked but not Cartesian. Then $x_1 \neq y_1$ and $x_2 \neq y_2$. Let $y' = (y_1, x_2)$ and $y'' = (x_1, y_2)$. If y' and y'' are both in $P(x)$, then $y \in P(x)$ by the copy consistency of F. So, without loss of generality, assume $y' \notin P(x)$.

If $\overline{N}(y) \subset \overline{N}(x)$, then $\overline{N}_1(y_1) \subset \overline{N}_1(x_1)$, since G_1 is S-thin and $x_1 \neq y_1$. Then we have

$$\begin{aligned}\overline{N}(y') &= \overline{N}_1(y_1) \times \overline{N}_2(x_2) \\ &\subset \overline{N}_1(x_1) \times \overline{N}_2(x_2) \\ &= \overline{N}(x).\end{aligned}$$

So, $y' \in R(x) \cap S(x)$. Also, $\overline{N}(y) \subset \overline{N}(x)$ implies $\overline{N}_2(y_2) \subset \overline{N}_2(x_2)$ since G_2 is S-thin and $x_2 \neq y_2$. Then

$$\begin{aligned}\overline{N}(y) &= \overline{N}_1(y_1) \times \overline{N}_2(y_2) \\ &\subset \overline{N}_1(y_1) \times \overline{N}_2(x_2) \\ &= \overline{N}(y').\end{aligned}$$

Since $x \to y$ is marked, $\overline{N}(y)$ must be maximal in $\mathcal{J}(x)$, but $\overline{N}(y) \subset \overline{N}(y')$ contradicts the maximality of $\overline{N}(y)$. Therefore, $x \to y$ is Cartesian.

Now we show that the set of all marked edges satisfies the copy consistency property. Suppose $u \to v$ is marked. Without loss of generality, we can assume that $u \to v$ is in a copy of G_1. Then $u = (u_1, u_2)$ and $v = (v_1, u_2)$, and $\overline{N}_1(v_1)$ is maximal in the set $\{\overline{N}_1(w_1) : (w_1, u_2) \in R(u) \cap S(u)\}$.

Consider another copy $u' \to v'$ of this edge. Then $u' = (u_1, u_2')$ and $v' = (v_1, u_2')$. Since $v \in R(u)$, $v' \in R(u')$ by the copy consistency of F. Because $v \in S(u)$, we also have $v' \in S(u')$ by the following argument:

$$\begin{aligned}\overline{N}(v) \subset \overline{N}(u) &\Rightarrow \overline{N}_1(v_1) \times \overline{N}_2(u_2) \subset \overline{N}_1(u_1) \times \overline{N}_2(u_2) \\ &\Rightarrow \overline{N}_1(v_1) \subset \overline{N}_1(u_1) \\ &\Rightarrow \overline{N}_1(v_1) \times \overline{N}_2(u_2') \subset \overline{N}_1(u_1) \times \overline{N}_2(u_2') \\ &\Rightarrow \overline{N}(v') \subset \overline{N}(u').\end{aligned}$$

Thus, $v' \in R(u') \cap S(u')$, and $u' \to v'$ is eligible to be marked.

Suppose there is a vertex $v'' = (v_1'', v_2'') \in R(u') \cap S(u')$ that prevents $u' \to v'$ from being marked. Such a v'' would have to satisfy the condition $\overline{N}(v') \subset \overline{N}(v'') \subset \overline{N}(u')$, or equivalently, $\overline{N}_1(v_1) \subset \overline{N}_1(v_1'') \subset \overline{N}_1(u_1)$. This equivalence holds by the following argument:

$$\begin{aligned} &\overline{N}_1(v_1) \times \overline{N}_2(u_2') \subset \overline{N}_1(v_1'') \times \overline{N}_2(v_2'') \subset \overline{N}_1(u_1) \times \overline{N}_2(u_2') \\ &\Leftrightarrow \overline{N}_2(u_2') = \overline{N}_2(v_2'') \\ &\Leftrightarrow u_2' = v_2'', \text{ since } G_2 \text{ is } S\text{-thin.} \end{aligned}$$

The statement $\overline{N}_1(v_1) \subset \overline{N}_1(v_1'') \subset \overline{N}_1(u_1)$ contradicts the maximality of $\overline{N}_1(v_1)$, unless $(v_1'', u_2) \notin R(u) \cap S(u)$. If that is the case, then either $(v_1'', u_2) \notin R(u)$ or $(v_1'', u_2) \notin S(u)$.

First suppose $(v_1'', u_2) \notin R(u)$, so then $(v_1'', u_2) \in P(u)$. By the copy consistency of F, we have $v'' = (v_1'', u_2') \in P(u')$. It follows that $v'' \notin R(u') \cap S(u')$, so v'' cannot prevent $u' \to v'$ from being marked.

Now suppose $(v_1'', u_2) \notin S(u)$. By the copy consistency of F, we have $v'' \notin S(u')$. Thus, $v'' \notin R(u') \cap S(u')$. Therefore, no such v'' exists. So, $u' \to v'$ is marked, and the set of marked edges is copy consistent. □

Lemma 3.4.2. *Assume the conditions of Lemma 3.4.1 hold with F closed under applications of Lemma 3.4.1, so that if $\overline{N}(y) \subset \overline{N}(x)$, then $y \in P(x)$. For all $x \in V(G)$, let $Q(x) = \overline{N}(x) \cap R(x)$, and for all $y \in Q(x)$, let $I(x,y) = \overline{N}(x) \cap \overline{N}(y)$ and $\mathcal{I}(x) = \{I(x,y) : y \in Q(x)\}$.*

Mark $x \to y$ if

i. $I(x,y)$ is strictly maximal in $\mathcal{I}(x)$ or

ii. $I(x,y)$ is maximal in $\mathcal{I}(x)$ and for all $y' \in Q(x)$ such that $I(x,y) = I(x,y')$, $\overline{N}(y') \not\subset \overline{N}(y)$.

Then all marked pairs are Cartesian and the set of all marked edges satisfies the copy consistency property.

Proof. We first prove that all marked pairs are Cartesian. Let $x = (x_1, x_2)$ and $y = (y_1, y_2)$, and suppose $x \to y$ is marked but not Cartesian. Then $x_1 \neq y_1$ and $x_2 \neq y_2$. Let $y' = (y_1, x_2)$ and $y'' = (x_1, y_2)$. By the copy consistency of F, $y \in P(x)$ if $y', y'' \in P(x)$, so assume $y' \notin P(x)$.

Let $z \in I(x,y) = \overline{N}(x) \cap \overline{N}(y)$. Then either $z = x$ or $x \to z$ and either $z = y$ or $y \to z$. By the definition of the strong product, it follows that $z \in \overline{N}(y')$. Thus, $z \in \overline{N}(x) \cap \overline{N}(y') = I(x,y')$. So, $I(x,y) \subseteq I(x,y')$.

If $I(x,y) \subsetneq I(x,y')$, then $x \to y'$ would be marked instead of $x \to y$. On the other hand, if $I(x,y) = I(x,y')$, then $\overline{N}(y') \subset \overline{N}(y)$ by the following argument:

$$
\begin{aligned}
&\overline{N}(x) \cap \overline{N}(y) = \overline{N}(x) \cap \overline{N}(y') \\
&\qquad \Rightarrow \big(\overline{N}_1(x_1) \times \overline{N}_2(x_2)\big) \cap \big(\overline{N}_1(y_1) \times \overline{N}_2(y_2)\big) \\
&\qquad\qquad = \big(\overline{N}_1(x_1) \times \overline{N}_2(x_2)\big) \cap \big(\overline{N}_1(y_1) \times \overline{N}_2(x_2)\big) \\
&\qquad \Rightarrow \big(\overline{N}_1(x_1) \cap \overline{N}_1(y_1)\big) \times \big(\overline{N}_2(x_2) \cap \overline{N}_2(y_2)\big) = \big(\overline{N}_1(x_1) \cap \overline{N}_1(y_1)\big) \times \overline{N}_2(x_2) \\
&\qquad \Rightarrow \overline{N}_2(x_2) \cap \overline{N}_2(y_2) = \overline{N}_2(x_2) \\
&\qquad \Rightarrow \overline{N}_2(x_2) \subseteq \overline{N}_2(y_2) \\
&\qquad \Rightarrow \overline{N}(y') = \overline{N}_1(y_1) \times \overline{N}_2(x_2) \subseteq \overline{N}_1(y_1) \times \overline{N}_2(y_2) = \overline{N}(y) \\
&\qquad \Rightarrow \overline{N}(y') \subset \overline{N}(y), \text{ since } y' \neq y \text{ and } G \text{ is } S\text{-thin.}
\end{aligned}
$$

But since $x \to y$ is marked, this contradicts the condition that if $I(x,y) = I(x,y')$, then $\overline{N}(y') \not\subset \overline{N}(y)$. Thus, $x \to y$ is Cartesian.

Now we prove copy consistency. Suppose $u \to v$ is marked and lies in a copy of G_1. Then $u = (u_1, u_2)$ and $v = (v_1, u_2)$. Let $u' \to v'$ be another copy of $u \to v$, so that $u' = (u_1, u_2')$ and $v' = (v_1, u_2')$. Note that $v' \in R(u') \cap S(u')$ by the same argument as in the proof of Lemma 3.4.1.

Suppose there is a $v'' = (v_1'', v_2'')$ such that $u' \to v''$ is chosen over $u' \to v'$. Then $v'' \in R(u') \cap S(u')$ and either $I(u',v') \subset I(u',v'')$, or $I(u',v') = I(u',v'')$ and for all $z \in Q(u')$ such that $I(u',v'') = I(u',z)$, $\overline{N}(z) \not\subset \overline{N}(v'')$.

First suppose that v'' is in the same G_1-copy as $u' \to v'$, so then $v'' = (v_1'', u_2')$. If $I(u',v') \subset$

$I(u', v'')$, then

$$\begin{aligned}(\overline{N}_1(u_1) \cap \overline{N}_1(v_1)) \times \overline{N}_2(u_2') \subset (\overline{N}_1(u_1) \cap \overline{N}_1(v_1'')) \times \overline{N}_2(u_2') \\ \Rightarrow \overline{N}_1(u_1) \cap \overline{N}_1(v_1) \subset \overline{N}_1(u_1) \cap \overline{N}_1(v_1'') \\ \Rightarrow (\overline{N}_1(u_1) \cap \overline{N}_1(v_1)) \times \overline{N}_2(u_2) \subset (\overline{N}_1(u_1) \cap \overline{N}_1(v_1'')) \times \overline{N}_2(u_2) \\ \Rightarrow I(u, v) \subset I(u, (v_1'', u_2)).\end{aligned}$$

Then $u \rightarrow (v_1'', u_2)$ would be marked instead of $u \rightarrow v$.

If $I(u', v') = I(u', v'')$, then since $u' \rightarrow v''$ is marked instead of $u' \rightarrow v'$, there exists a $z' = (z_1, z_2) \in Q(u')$ such that $z' \neq v'$, $I(u', v') = I(u', z')$, and $\overline{N}(z') \subset \overline{N}(v')$. Then

$$\begin{aligned}I(u', v') = I(u', z') &\Rightarrow \overline{N}_2(u_2') = \overline{N}_2(u_2') \cap \overline{N}_2(z_2) \\ &\Rightarrow \overline{N}_2(u_2') \subseteq \overline{N}_2(z_2).\end{aligned}$$

We also have $\overline{N}(z') \subset \overline{N}(v')$, which implies that $\overline{N}_2(z_2) \subseteq \overline{N}_2(u_2')$. Thus, $\overline{N}_2(z_2) = \overline{N}_2(u_2')$, and since G_2 is S-thin, $z_2 = u_2'$. Then we have $z_1 \neq v_1$.

Let $z = (z_1, u_2)$. Since $\overline{N}(z') \subset \overline{N}(v')$ and G_1 is S-thin, we have $\overline{N}_1(z_1) \subset \overline{N}_1(v_1)$. Also,

$$\begin{aligned}z' \in Q(u') &\Rightarrow z' \in \overline{N}(u') \\ &\Rightarrow z_1 \in \overline{N}_1(u_1) \\ &\Rightarrow z \in \overline{N}(u).\end{aligned}$$

If $z \in P(u)$, then z' would be in $P(u')$ by the copy consistency of H. But, $z' \in R(u')$, so $z \in R(u)$. Thus, $z \in Q(u)$. Also, $I(u, v') = I(u', z') \Rightarrow \overline{N}_1(u_1) \cap \overline{N}_1(v_1) = \overline{N}_1(u_1) \cap \overline{N}_1(z_1)$. Then

$$\begin{aligned}I(u, v) &= (\overline{N}_1(u_1) \cap \overline{N}_1(v_1)) \times \overline{N}_2(u_2) \\ &= (\overline{N}_1(u_1) \cap \overline{N}_1(z_1)) \times \overline{N}_2(u_2) \\ &= I(u, z).\end{aligned}$$

Also, $\overline{N}(z) = \overline{N}_1(z_1) \times \overline{N}_2(u_2) \subset \overline{N}_1(v_1) \times \overline{N}_2(u_2) = \overline{N}(v)$, which means that $u \rightarrow v$ would not be marked.

Now suppose that v'' is not in the same copy of G_1 as $u' \to v'$, so then $v_2'' \neq u_2'$. Note that $I(u', v') \subseteq I(u', v'')$ implies $\overline{N}_2(u_2') \subset \overline{N}_2(v_2'')$, since G_2 is S-thin.

Then $\overline{N}(u') = \overline{N}_1(u_1) \times \overline{N}_2(u_2') \subset \overline{N}_1(u_1) \times \overline{N}_2(v_2'') = \overline{N}(u_1, v_2'')$. This implies that $(u_1, v_2'') \in P(u')$ since F is closed under applications of Lemma 3.4.1. Since $v'' \notin P(u')$, we can assume $v_1'' \neq u_1$. Thus, we have

$$\begin{aligned} I(u', v'') &= \left(\overline{N}_1(u_1) \times \overline{N}_2(u_2')\right) \cap \left(\overline{N}_1(v_1'') \times \overline{N}_2(v_2'')\right) \\ &= \left(\overline{N}_1(u_1) \cap \overline{N}_1(v_1'')\right) \times \left(\overline{N}_2(u_2') \cap \overline{N}_2(v_2'')\right) \\ &= \left(\overline{N}_1(u_1) \cap \overline{N}_1(v_1'')\right) \times \overline{N}_2(u_2'), \text{ since } \overline{N}_2(u_2') \subset \overline{N}_2(v_2'') \\ &= I(u', (v_1'', u_2')). \end{aligned}$$

Also, $\overline{N}(v_1'', u_2') = \overline{N}_1(v_1'') \times \overline{N}_2(u_2') \subset \overline{N}_1(v_1'') \times \overline{N}_2(v_2'') = \overline{N}(v'')$, but this contradicts $u' \to v''$ being marked unless $(v_1'', u_2') \in P(u')$. Then by the copy consistency of F, $(u_1, v_2''), (v_1'', u_2') \in P(u')$ implies that $v'' \in P(u')$, so no such v'' exists. Therefore, the set of marked edges is copy consistent. □

3.5 Constructing the Cartesian Skeleton

The *Cartesian skeleton* H of a digraph G is the subdigraph containing the edges of G which must be Cartesian with respect to any decomposition of G under the strong direct product. To be precise, if $H = H_1 \,\square\, H_2$ and $G = G_1 \boxtimes G_2$, then for every $x \in V(G)$, $V(H_i^x) = V(G_i^x)$. In this section, we give an algorithm to construct the Cartesian skeleton of an S-thin digraph with no complete factors. This algorithm is modeled after the marking algorithms of Feigenbaum and Schäffer (9) and Imrich (10). Following Feigenbaum and Schäffer, all of the edges marked in the algorithm are indeed edges of the input graph G.

Algorithm 1. MARK(G)

For each $x \in V(G)$

$P(x) \leftarrow \{x\}$.

Insert $P(x)$ into $\mathcal{P}$.

$S(x) \leftarrow \{y : \overline{N}(y) \subset \overline{N}(x)\}$.

M1: While there is an $x \in V(G)$ such that $R(x) \cap S(x) \neq \emptyset$

For each such x

$\mathcal{J}(x) \leftarrow \{\overline{N}(y) : y \in R(x) \cap S(x)\}$.

If $\overline{N}(y)$ is maximal in $\mathcal{J}(x)$, then mark $x \rightarrow y$.

If $x \rightarrow y$ was marked, then replace $P(x)$ and $P(y)$ with $P(x) \cup P(y)$ in $\mathcal{P}$.

End **M1**

M2: While $|\mathcal{P}| > 1$

M3: For each $x \in V(G)$

$Q(x) \leftarrow \overline{N}(x) \cap R(x)$.

If $Q(x) \neq \emptyset$, then

For each $y \in Q(x)$, $I(x,y) \leftarrow \overline{N}(x) \cap \overline{N}(y)$.

$\mathcal{I}(x) \leftarrow \{I(x,y) : y \in Q(x)\}$.

If $I(x,y)$ is strictly maximal in $\mathcal{I}(x)$, then mark $x \rightarrow y$.

If $I(x,y)$ is non-strictly maximal in $\mathcal{I}(x)$ and for all $y' \in Q(x)$

with $I(x,y) = I(x,y')$, $\overline{N}(y') \not\subset \overline{N}(y)$, then mark $x \rightarrow y$.

If $x \rightarrow y$ was marked, then replace $P(x)$ and $P(y)$ with $P(x) \cup P(y)$ in $\mathcal{P}$.

End **M3**

End **M2**

Note that Lemma 3.4.1 shows the edges marked in loop M1 are Cartesian and the set of marked edges satisfies the copy consistency property. By Lemma 3.4.2, the edges marked in loop M2 are also Cartesian and the set of marked edges satisfies the copy consistency property.

Lemma 3.5.1. *All iterations of M1 and M2, except the ones in which the loops are terminated, reduce the size of* $\mathcal{P}$.

Proof. To show this for the loop M1, suppose there is an $x \in V(G)$ such that $R(x) \cap S(x) \neq \emptyset$. At least one set in $\mathcal{J}(x)$ must be maximal, so at least one edge $x \rightarrow y$ is marked in this iteration. Since $y \in R(x)$, $y \notin P(x)$ at the beginning of the iteration, and then $y \in P(x)$ at the end of the iteration. Thus, the size of $\mathcal{P}$ is reduced.

For M2, suppose $|\mathcal{P}| > 1$. Since G is weakly connected, there is an $x \in V(G)$ with at least one neighbor which is not in $P(x)$. So, $Q(x) = \overline{N}(x) \cap R(x) \neq \emptyset$. If $\mathcal{I}(x)$ has a strictly maximal element $I(x, y)$, then $x \to y$ is marked and the size of $\mathcal{P}$ is reduced. Otherwise, if $\mathcal{I}(x)$ has no strictly maximal element, then because G is S-thin, there is a $y \in V(G)$ such that $I(x, y)$ is maximal and y has a strictly minimal closed neighborhood. Then $x \to y$ is marked, and the size of $\mathcal{P}$ is reduced. □

Assuming $|V(G)| = n$, determining the closed neighborhood of a vertex by checking the adjacency matrix of G has complexity $O(n)$, and an edge can be marked in constant time (11). The partition can also be constructed in polynomial time (5). The operations of finding intersections of sets, checking set inclusions, and determining maximal subsets can all be done in polynomial time, so all of the operations inside the loops M1 and M2 can be completed in time polynomial in n. Since the size of $\mathcal{P}$ is reduced for each iteration of M1 and M2, the time complexity of the entire algorithm is polynomial in n.

Lemma 3.5.2. *Let G be a weakly connected S-thin digraph. Then there exists a weakly connected digraph H defined on the same vertices of G whose edges are Cartesian and copy consistent with respect to any decomposition of G as a strong product.*

Proof. Let H be the digraph whose edge set consists of the edges marked in Algorithm 1. Since M2 terminates when $|\mathcal{P}| = 1$, H is weakly connected. H is constructed without reference to any particular strong product decomposition of G, and the decomposition $G = G_1 \boxtimes G_2$ in Lemma 3.4.1 and Lemma 3.4.2 was arbitrary. Thus, the edges of H are Cartesian and copy consistent with respect to any decomposition of G as a strong product. □

3.6 Unique Factorization of S-thin Digraphs

In this section, we show that the strong product factorization of weakly connected, simple directed graphs is unique. We also show that this factorization can be computed in polynomial time.

Suppose digraph G has the factorization $G = G_1 \boxtimes G_2 \boxtimes \cdots \boxtimes G_k$, and let H be the digraph with $V(H) = V(G)$ and $E(H) = \text{MARK}(G)$. Let H_i for $i = 1, \ldots, k$ be defined as follows:

$$V(H_i) = V(G_i);$$

$$E(H_i) = \{x_i \to y_i : (x_1, x_2, \ldots, x_k) \to (y_1, y_2, \ldots, y_k) \in E(H)\}.$$

Then $H = H_1 \square H_2 \square \cdots \square H_k$. From Feigenbaum, we know that H has a unique prime factor decomposition with respect to the Cartesian product (8). Let $H = Q_1 \square Q_2 \square \cdots \square Q_m$ be this decomposition. We use $\prod^{\square}$ to denote the Cartesian product. There exist disjoint sets $I_1, I_2, \ldots, I_k$ such that $\bigcup_{i=1}^{k} I_i = \{1, 2, \ldots, m\}$ and $H_i = \prod_{j \in I_i}^{\square} Q_j$, for $i = 1, 2, \ldots, k$. We also have $H_i^x = \left(\prod_{j \in I_i}^{\square} Q_j\right)^x$, for all $x \in V(G)$ and $i = 1, 2, \ldots, k$, by the unique coordinatization.

Lemma 3.6.1. *Let G be a weakly connected S-thin digraph, and let $A \boxtimes B$ and $C \boxtimes D$ be two decompositions of G. Then there exists a decomposition $A_C \boxtimes A_D \boxtimes B_C \boxtimes B_D$ of G such that $A = A_C \boxtimes A_D$, $B = B_C \boxtimes B_D$, $C = A_C \boxtimes B_C$, and $D = A_D \boxtimes B_D$.*

Proof. Let $Q_1 \square Q_2 \square \cdots \square Q_k$ be the unique prime factor decomposition of the digraph H constructed by MARK(G). Let $I_A \subseteq \{1, 2, \ldots, k\}$ with $V(A) = V\left(\prod_{j \in I_A}^{\square} Q_i\right)$, and let I_B, I_C, and I_D be defined analogously. Set $H_{A,C} = \prod_{i \in I_A \cap I_C}^{\square} Q_i$, and define $H_{A,D}$, $H_{B,C}$, and $H_{B,D}$ similarly. Then $H = H_{A,C} \square H_{A,D} \square H_{B,C} \square H_{B,D}$. So, from now on, we will use only four coordinates (x_1, x_2, x_3, x_4) for every vertex $x \in V(G)$.

It is possible that not all of the four intersections $I_A \cap I_C$, $I_A \cap I_D$, $I_B \cap I_C$, and $I_B \cap I_D$ are nonempty. Suppose, for example, that $I_B \cap I_D = \emptyset$. Then $I_A \cap I_D \neq \emptyset$ and $I_B \cap I_C \neq \emptyset$. If $I_A \cap I_C = \emptyset$, then $I_A = I_D$ and thus, $I_B = I_C$. But then there is nothing to prove, so we can assume that all but possibly $I_B \cap I_D$ are nonempty. Then at least three of the four coordinates are nontrivial, but it is possible that all of the vertices have the same fourth coordinate.

Define A_C as $p_1(G)$, so that $V(A_C) = V(H_{A,C})$ and $x_1 \to y_1 \in E(A_C)$ if there are $x = (x_1, x_2, x_3, x_4)$ and $y = (y_1, y_2, y_3, y_4)$ in $V(G)$ such that $x \to y \in E(G)$. Similarly, define $A_D = p_2(G)$, $B_C = p_3(G)$, and $B_D = p_4(G)$. If all of the vertices of G have the same fourth

coordinate, then $B_D = K_1$, or in other words, B_D is the unit graph with respect to strong direct multiplication. For the remainder of the proof, it suffices to show that $A = A_C \boxtimes A_D$.

Let p_A denote the projection of G onto the vertex set of A, and define p_B, p_C, and p_D in the same manner. Thus, we have

$$p_A(x_1, x_2, x_3, x_4) = (x_1, x_2, -, -),$$
$$p_B(x_1, x_2, x_3, x_4) = (-, -, x_3, x_4),$$
$$p_C(x_1, x_2, x_3, x_4) = (x_1, -, x_3, -),$$
$$p_D(x_1, x_2, x_3, x_4) = (-, x_2, -, x_4).$$

To prove $A = A_C \boxtimes A_D$, it suffices to show that $p_A(x) \to p_A(y) \in E(A)$ if and only if $p_1(x) \to p_1(y) \in E(A_C)$ and $p_2(x) \to p_2(y) \in E(A_D)$.

Suppose $p_A(x) \to p_A(y) \in E(A)$. Without loss of generality, we can assume $x \to y \in E(G)$. Then $p_1(x) \to p_1(y) \in E(A_C)$ and $p_2(x) \to p_2(y) \in E(A_D)$ by the definition of A_C and A_D.

For the other direction, suppose $p_1(x) \to p_1(y) \in E(A_C)$ and $p_2(x) \to p_2(y) \in E(A_D)$. In other words,

$$(x_1, -, -, -) \to (y_1, -, -, -) \in E(A_C)$$

and

$$(-, x_2, -, -) \to (-, y_2, -, -) \in E(A_D).$$

Then there are vertices $x' = (x_1, a_2', a_3', a_4')$, $y' = (y_1, b_2', b_3', b_4')$, $x'' = (a_1'', x_2, a_3'', a_4'')$, and $y'' = (b_1'', x_2, b_3'', b_4'')$ in G with $x' \to y'$ and $x'' \to y''$ in $E(G)$.

Thus, $(x_1, -, a_3', -) \to (y_1, -, b_3', -) \in E(C)$ and $(-, x_2, -, a_4'') \to (-, y_2, -, b_4'') \in E(D)$. Since $G = C \boxtimes D$, we have $(x_1, x_2, a_3', a_4'') \to (y_1, y_2, b_3', b_4'') \in E(G)$. Therefore, $(x_1, x_2, -, -) \to (y_1, y_2, -, -) \in E(A)$, so $p_A(x) \to p_A(y) \in E(A)$. □

The decomposition $A_C \boxtimes A_D \boxtimes B_C \boxtimes B_D$ in Lemma 3.6.1 is called a *common refinement* of the products $A \boxtimes B$ and $C \boxtimes D$. We say the digraph G satisfies the *refinement property* if any two such factorizations of G have a common refinement.

Lemma 3.6.2. *Every weakly connected, S-thin digraph G has a unique prime factor decomposition with respect to the strong product.*

Proof. We proceed by induction on the number of vertices of G, $n = |V(G)|$. For $n = 1$, clearly G has a UPFD. Suppose Lemma 3.6.2 holds for all digraphs with fewer than n vertices. Let $G_1 \boxtimes G_2 \boxtimes \cdots \boxtimes G_r = Q_1 \boxtimes Q_2 \boxtimes \cdots \boxtimes Q_s$ be two prime factorizations of G. Then there exist digraphs B and D such that $G \cong G_1 \boxtimes B \cong Q_1 \boxtimes D$.

By Lemma 3.6.1, taking $A \cong G_1$ and $C \cong Q_1$, we have $G \cong A_C \boxtimes A_D \boxtimes B_C \boxtimes B_D$, with $G_1 \cong A_C \boxtimes A_D$, $B \cong B_C \boxtimes B_D$, $Q_1 \cong A_C \boxtimes B_C$, and $D \cong A_D \boxtimes B_D$. Since G_1 is prime, either $G_1 \cong A_C$ or $G_1 \cong A_D$. First suppose $G_1 \cong A_C$. Then $A_D \cong K_1$ and $D \cong B_D$. Since A_C is nontrivial and Q_1 is prime, $Q_1 \cong A_C \cong G_1$ and $B_C \cong K_1$. Then $B \cong B_C \boxtimes B_D \cong B_D$, so $B \cong D$. By the induction hypothesis, both B and D have unique prime factorizations, so $r = s$ and $G_i \cong Q_i$ for $2 \leq i \leq r$.

Now suppose $G_1 \cong A_D$. Then since G_1 is prime, $A_C \cong K_1$, and thus, $Q_1 \cong B_C$. Also,

$$G_2 \boxtimes G_3 \boxtimes \cdots \boxtimes G_r \cong B \cong B_C \boxtimes B_D \cong Q_1 \boxtimes B_D$$

and

$$Q_2 \boxtimes Q_3 \boxtimes \cdots \boxtimes Q_s \cong D \cong A_D \boxtimes B_D \cong G_1 \boxtimes B_D.$$

By the induction hypothesis, both B and D have UPFD's, so without loss of generality, assume $Q_1 \cong G_2$. Then $B_D \cong G_3 \boxtimes \cdots \boxtimes G_r$, so $D \cong G_1 \boxtimes B_D \cong G_1 \boxtimes G_3 \boxtimes \cdots \boxtimes G_r$. Thus,

$$G \cong G_1 \boxtimes B \cong G_1 \boxtimes Q_1 \boxtimes B_D \cong Q_1 \boxtimes G_1 \boxtimes B_D \cong Q_1 \boxtimes D \cong G_2 \boxtimes D \cong G.$$

Therefore, G has a unique prime factor decomposition. □

Lemma 3.6.3. *The prime factor decomposition of weakly connected, S-thin digraphs with respect to the strong product can be found in polynomial time.*

Proof. Let G be a weakly connected S-thin digraph. The Cartesian skeleton H of G can be found in polynomial time using Algorithm 1. Also, the UPFD of H, $H_1 \square H_2 \square \cdots \square H_k$,

can be found in polynomial time using the Cartesian factorization for digraphs presented by Feigenbaum (8).

Let $G = G_1 \boxtimes G_2 \boxtimes \cdots \boxtimes G_r$ be the UPFD of G. There exists a partition $I_1, I_2, \ldots, I_r$ of $I = \{1, 2, \ldots, k\}$ such that $V(G_i^x) = V\Big(\Big(\prod_{j \in I_i}^{\square} H_j\Big)^x\Big)$ for all $x \in V(G)$ and for $1 \leq i \leq r$. To find the partition, let J be any subset of I. Define digraphs A and B by the projections $p_J(G)$ and $p_{I \setminus J}(G)$ onto the vertex sets $V\Big(\prod_{i \in J}^{\square} H_i\Big)$ and $V\Big(\prod_{i \in I \setminus J}^{\square} H_i\Big)$. If $J = I_i$ for some i or if J is the union of some of the I_i's, then $G = A \boxtimes B$. In general, since $E(G) \subseteq E(A \boxtimes B)$, $G = A \boxtimes B$ if and only if $|E(G)| = |E(A \boxtimes B)|$.

H_i is nontrivial for all i, so $k \leq \log_2 n$. Therefore, I has at most $2^{\log_2 n} = n$ subsets. Construction of A and B has complexity $O(m \log n)$, where $m = |E(G)|$. Thus, we can find a minimal subset J of I such that $G = A \boxtimes B$ in polynomial time. Then $A = G_i$ for some i, and $B = \prod_{\substack{1 \leq j \leq r \\ j \neq i}} G_j$. Repeating this procedure at most $\log n$ times decomposes G into its prime factors. □

3.7 Factoring Weakly Connected Digraphs

Once we have the factorization of G/S, the factorization of G can be retrieved by examining the sizes of the equivalence classes of the factors of G/S.

Lemma 3.7.1. *Suppose a digraph G with no complete factors is a strong product graph $G = G_1 \boxtimes G_2$, and suppose the decomposition $G/S = G_1/S \boxtimes G_2/S$ is known. Then G_1 and G_2 can be determined in polynomial time.*

Proof. Let $x = (x_1, x_2) \in G_1/S \times G_2/S$, and let $\left|\overline{(x_1, x_2)}\right|$ be the size of the S-equivalence class of G that is mapped into x in $V(G_1/S \boxtimes G_2/S)$. Let $|\overline{x_1}|$ be the size of the S-equivalence class of G_1 that is mapped into x_1 in $V(G_1/S)$, and $|\overline{x_2}|$ be the size of the S-equivalence class of G_2 that is mapped into x_2 in $V(G_2/S)$. Then $\left|\overline{(x_1, x_2)}\right| = |\overline{x_1}| \cdot |\overline{x_2}|$. Since G is not $\boxtimes$-divisible by K_k for any $k > 1$, $\gcd\{|\overline{y}| : y \in V(G_2/S)\} = 1$. Thus,

$$|\overline{x_1}| = \gcd\{|\overline{x_1}| \cdot |\overline{y}| : y \in V(G_2/S)\} = \gcd\left\{\left|\overline{(x_1, y)}\right| : y \in V(G_2/S)\right\}.$$

Similarly,

$$|\overline{x_2}| = \gcd\{|\overline{y}| \cdot |\overline{x_2}| : y \in V(G_1/S)\} = \gcd\left\{\left|\overline{(y, x_2)}\right| : y \in V(G_1/S)\right\}.$$

To determine G_1, replace each vertex $x_1 \in V(G_1/S)$ with the complete graph $K_{|\overline{x_1}|}$. Note that if $|\overline{x_1}| = 1$, then the vertex x_1 remains unchanged. Then if $x_1 \to y$ or $y \to x_1$ in G_1/S, add the corresponding edges $z \to y$ or $y \to z$ for all $z \in K_{|\overline{x_1}|}$. When this procedure is completed, the resulting digraph will be G_1. In the same manner, G_2 can be determined.

To see that G_1 and G_2 can be determined in polynomial time, first note that the greatest common divisor of a set of size n can be computed in time polynomial in $\log n$ (5). Then $|\overline{x_1}|$ can be computed in time polynomial in $\log |G_2/S|$. Since $|G_2/S| \leq |G_2|$, clearly, $|\overline{x_1}|$ can be computed in time polynomial in $n = |V(G)|$. The same holds for $|\overline{x_2}|$. Edges can be inserted in constant time (11). Thus, the digraphs G_1 and G_2 can be determined in polynomial time. □

Lemma 3.7.2. *Let G be a weakly connected digraph with no complete factors. Then G satisfies the refinement property. In other words, if $A \boxtimes B$ and $C \boxtimes D$ are two decompositions of G with respect to the strong product, for which $A/S \boxtimes B/S$ and $C/S \boxtimes D/S$ are distinct decompositions of G/S, then there exists a decomposition $G = A_C \boxtimes A_D \boxtimes B_C \boxtimes B_D$ such that $A = A_C \boxtimes A_D$, $B = B_C \boxtimes B_D$, $C = A_C \boxtimes B_C$, and $D = A_D \boxtimes B_D$.*

Proof. By Lemma 3.6.1, G/S satisfies the refinement property, so $A/S \boxtimes B/S$ and $C/S \boxtimes D/S$ have a common refinement. Suppose $A'_C \boxtimes A'_D \boxtimes B'_C \boxtimes B'_D$ is this refinement, where $A/S = A'_C \boxtimes A'_D$, $B/S = B'_C \boxtimes B'_D$, $C/S = A'_C \boxtimes B'_C$, and $D/S = A'_D \boxtimes B'_D$. Let (x, y, u, v) be the coordinatization corresponding to this decomposition. Then there exist functions $a(x, y)$, $b(u, v)$, $c(x, u)$, and $d(y, v)$, where $a(x, y)$ is the size of the S-class of A mapped into the vertex $(x, y) \in V(A/S)$, and the other functions are defined in a similar manner.

We have $a(x, y)b(u, v) = c(x, u)d(y, v)$. We need to show there exist functions $a_1(x)$, $a_2(y)$, $b_1(u)$, and $b_2(v)$ such that $a(x, y) = a_1(x)a_2(y)$, $b(u, v) = b_1(u)b_2(v)$, $c(x, u) = a_1(x)b_1(u)$, and $d(y, v) = a_2(y)b_2(v)$. Also, we need to show that $\gcd\{a_1(x) : x \in V(A'_C)\} = 1$ and that analogous properties hold for a_2, b_1, and b_2.

Since $a(x,y)b(u,v) = c(x,u)d(y,v)$, we have $\frac{a(x,y)}{d(y,v)} = \frac{c(x,u)}{b(u,v)}$, and both sides depend only on x and v. Then $\frac{a(x,y)}{d(y,v)} = \frac{a(x,y_0)}{d(y_0,v)}$, and thus, $\frac{a(x,y)}{a(x,y_0)} = \frac{d(y,v)}{d(y_0,v)}$. Note that both fractions depend only on y and y_0, so there is a function $f(y,y_0) = \frac{d(y,v)}{d(y_0,v)}$ such that $a(x,y) = a(x,y_0)f(y,y_0)$. Since y_0 was arbitrarily fixed, we can write $a(x,y) = a_1(x)a_2(y)$. In a similar manner, the functions b, c, and d can be decomposed. Then

$$a_1(x)a_2(y)b_1(u)b_2(v) = c_1(x)c_2(u)d_1(y)d_2(v),$$

so there exist constants k_1, k_2, k_3, k_4 such that $k_1a_1(x) = c_1(x)$, $k_2a_2(y) = d_1(y)$, $k_3b_1(u) = c_2(u)$, $k_4b_2(v) = d_2(v)$, and $k_1k_2k_3k_4 = 1$.

Clearly, a_i, b_i, c_i, d_i, $i = 1, 2$, can be chosen to be rational functions, but we would like them to be integer functions. Consider

$$\frac{\text{numerator}(a_1(x))}{\text{denominator}(a_1(x))} \cdot \frac{\text{numerator}(a_2(y))}{\text{denominator}(a_2(y))} = a_1(x) \cdot a_2(y) = a(x,y).$$

Assuming all fractions to be in lowest terms, since $a(x,y)$ is an integer, the denominator of $a_1(x)$ divides the numerator of $a_2(y)$, and the denominator of $a_2(y)$ divides the numerator of $a_1(x)$. This is true for arbitrary x and y. Let n_1 be the least common multiple of $\{\text{denominator}(a_1(x))\}$ and n_2 the least common multiple of $\{\text{denominator}(a_2(y))\}$. Then n_1 divides the numerator of every $a_2(y)$, and n_2 divides the numerator of every $a_1(x)$. So, we can write $a_1(x) = \frac{a_1'(x)}{n_1}$ and $a_2(y) = \frac{a_2'(y)}{n_2}$. Then

$$\frac{a_1'(x)}{n_1} \cdot \frac{a_2'(y)}{n_2} = \frac{a_1'(x)}{n_2} \cdot \frac{a_2'(y)}{n_1} = a(x,y).$$

Replacing $a_1(x)$ by $\frac{a_1'(x)}{n_2}$ and $a_2(y)$ by $\frac{a_2'(y)}{n_1}$, we have an integer factorization of $a(x,y)$. The same procedure can be done for the functions b,c, and d. Then $k_i = 1$ for $i = 1, 2, 3, 4$.

Now consider the greatest common divisor. If $\gcd\{a_1(x) : x \in V(A_C')\} \neq 1$, then $\gcd\{(x,y) : (x,y) \in V(A)\} \neq 1$, which implies that A has a complete factor. But A has no complete factors, so it must be the case that $\gcd\{a_1(x) : x \in V(A_C')\} = 1$. A similar argument holds for a_2, b_1, and b_2. □

We are now ready for the main result.

Theorem 3.7.3. *Let G be a weakly connected digraph. Then G has a unique prime factor decomposition with respect to the strong product. Moreover, this decomposition can be determined in polynomial time.*

Proof. Let G be a finite, weakly connected digraph. In Section 3.3, we showed how to find the largest complete factor K_k of G. This complete graph can be factored in time polynomial in k by finding the prime factorization $p_1 p_2 \cdots p_t$ of k. Then we can express G as the product $G = Q \boxtimes K_{p_1} \boxtimes K_{p_2} \boxtimes \cdots \boxtimes K_{p_t}$, where the digraph Q has no complete factors. By Lemma 3.3.5, Q is uniquely determined.

It remains to be shown that such a digraph Q has a unique prime factorization. Suppose $G_1 \boxtimes G_2 \boxtimes \cdots \boxtimes G_r$ is a prime factorization of Q. By Lemma 3.6.2, Q/S has a UPFD, so let $Q/S = Q_1 \boxtimes Q_2 \boxtimes \cdots \boxtimes Q_k$ be this unique prime factorization. Then there is a partition $\mathcal{I} = \{I_1, I_2, \ldots, I_r\}$ of the index set $I = \{1, 2, \ldots, k\}$ such that $G_i/S = \prod_{j \in I_i} Q_j$.

Suppose $G'_1 \boxtimes G'_2 \boxtimes \cdots \boxtimes G'_s$ is another prime factorization of Q. Similarly, there is a partition $\mathcal{I}' = \{I'_1, I'_2, \ldots, I'_s\}$ of I such that $G'_i/S = \prod_{j \in I'_i} Q_j$. If $\mathcal{I}' \neq \mathcal{I}$, then by Lemma 3.7.2 there would be a refinement of the product. Since all of the G_i and G'_i factors are prime, that is not possible. Thus, the prime factorization of Q is unique.

Now consider the complexity of finding the unique prime factor decomposition of G. The factorization is found by completing the following steps:

1. Determine S and G/S.
2. Write G as the product $Q \boxtimes K_{p_1} \boxtimes K_{p_2} \boxtimes \cdots \boxtimes K_{p_t}$, where Q has no complete factors.
3. Construct the Cartesian skeleton H of Q/S using Algorithm 1.
4. Factor H with respect to the Cartesian product.
5. Determine the prime factors of Q/S.
6. Determine the prime factors of Q.

Step 1 has complexity $O(n^3)$ by Lemma 3.2.1. The second step was shown to have polynomial complexity in Section 3.3. By Lemma 3.6.3, steps 3-5 can be completed in polynomial

time. Finally, the last step can be completed by repeated applications of Lemma 3.7.1. To get the prime factors of Q, find all minimal subsets J of $I = \{1, 2, \ldots, k\}$ such that there are graphs A and B with $G = A \boxtimes B$, $A/S = \prod_{i \in J} Q_i$, and $B/S = \prod_{i \in I \setminus J} Q_j$. Since J is minimal, by the refinement of Lemma 3.7.2, A must be prime. □

3.8 An Example

In this section, we present an example to visualize how the factoring algorithm works. Consider the digraph G in Figure 3.1. Note that G is S-thin and has no complete factors, so we begin by constructing the Cartesian skeleton H using Algorithm 1.

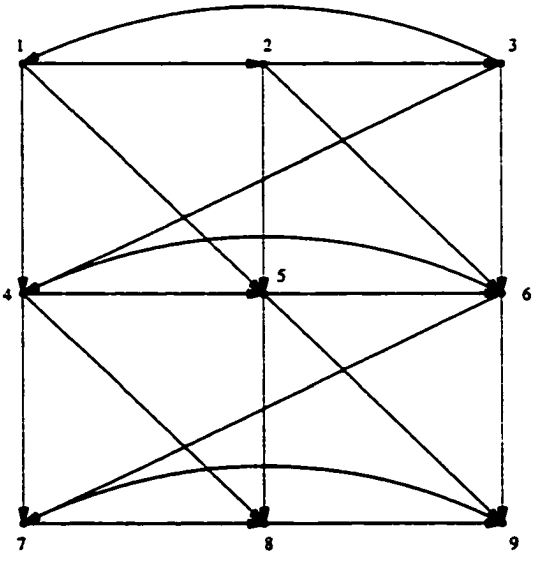

Figure 3.1 The digraph G

We first determine the closed neighborhood of each vertex:

$$\overline{N}(1) = \{1, 2, 4, 5\} \qquad \overline{N}(2) = \{2, 3, 5, 6\} \qquad \overline{N}(3) = \{1, 3, 4, 6\}$$

$$\overline{N}(4) = \{4, 5, 7, 8\} \qquad \overline{N}(5) = \{5, 6, 8, 9\} \qquad \overline{N}(6) = \{4, 6, 7, 9\}$$

$$\overline{N}(7) = \{7, 8\} \qquad \overline{N}(8) = \{8, 9\} \qquad \overline{N}(9) = \{7, 9\}$$

The partition $\mathcal{P}$ is initialized as $\{\{1\},\{2\},\{3\},\{4\},\{5\},\{6\},\{7\},\{8\},\{9\}\}$, and the sets $S(x)$ are constructed for each vertex x:

$$S(1) = S(2) = S(3) = S(7) = S(8) = S(9) = \emptyset$$

$$S(4) = \{7\} \qquad S(5) = \{8\} \qquad S(6) = \{9\}$$

In loop M1, the only nonempty sets $\mathcal{J}(x)$ are $\mathcal{J}(4) = \{\overline{N}(7)\}, \mathcal{J}(5) = \{\overline{N}(8)\}$, and $\mathcal{J}(6) = \{\overline{N}(9)\}$. So, the edges $4 \to 7, 5 \to 8$, and $6 \to 9$ are marked. At the end of M1, $\mathcal{P} = \{\{1\},\{2\},\{3\},\{4,7\},\{5,8\},\{6,9\}\}$.

In loop M2, the sets $Q(x)$ are constructed for each vertex x:

$$Q(1) = \{2,4,5\} \qquad Q(2) = \{3,5,6\} \qquad Q(3) = \{1,4,6\}$$
$$Q(4) = \{5,8\} \qquad Q(5) = \{6,9\} \qquad Q(6) = \{4,7\}$$
$$Q(7) = \{8\} \qquad Q(8) = \{9\} \qquad Q(9) = \{7\}$$

The sets $I(x,y)$ are also determined for each $y \in Q(x)$:

$$I(1,2) = \{2,5\} \qquad I(1,4) = \{4,5\} \qquad I(1,5) = \{5\}$$
$$I(2,3) = \{3,6\} \qquad I(2,5) = \{5,6\} \qquad I(2,6) = \{6\}$$
$$I(3,1) = \{1,4\} \qquad I(3,4) = \{4\} \qquad I(3,6) = \{4,6\}$$
$$I(4,5) = \{5,8\} \qquad I(4,8) = \{8\} \qquad I(5,6) = \{6,9\}$$
$$I(5,9) = \{9\} \qquad I(6,4) = \{4,7\} \qquad I(6,7) = \{7\}$$
$$I(7,8) = \{8\} \qquad I(8,9) = \{9\} \qquad I(9,7) = \{7\}$$

Then by strict maximality, the following edges are marked: $1 \to 2$, $1 \to 4$, $2 \to 3$, $2 \to 5$, $3 \to 1$, $3 \to 6$, $4 \to 5$, $5 \to 6$, $6 \to 4$, $7 \to 8$, $8 \to 9$, and $9 \to 7$. At the end of the first iteration, $\mathcal{P} = \{1,2,3,4,5,6,7,8,9\}$, so loop M2 is terminated.

Figure 3.2 shows the digraph $H = \text{MARK}(G)$. The solid edges were marked in loop M1 of the algorithm, and the dashed edges were marked in loop M2. Note that all of the edges are Cartesian and that H is a subdigraph of G.

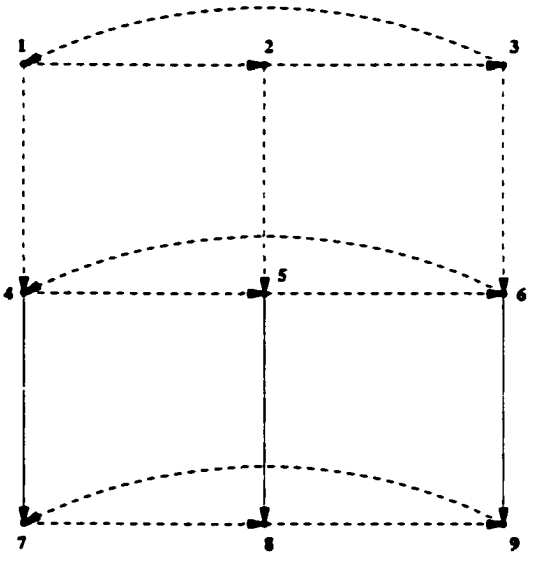

Figure 3.2 The digraph $H = \text{MARK}(G)$

The digraph H is then factored with respect to the Cartesian product. Figure 3.3 shows this factorization. We can then retrieve the strong factorization of G, seen in Figure 3.4. In this example, the factors of H and G are exactly the same. This might not happen in general because a factor of G could be prime with respect to the strong product but reducible under the Cartesian product. In that case, two or more of the Cartesian factors of H will be combined into one factor of G. More generally, G itself could be prime with respect to the strong product even if H is reducible under the Cartesian product.

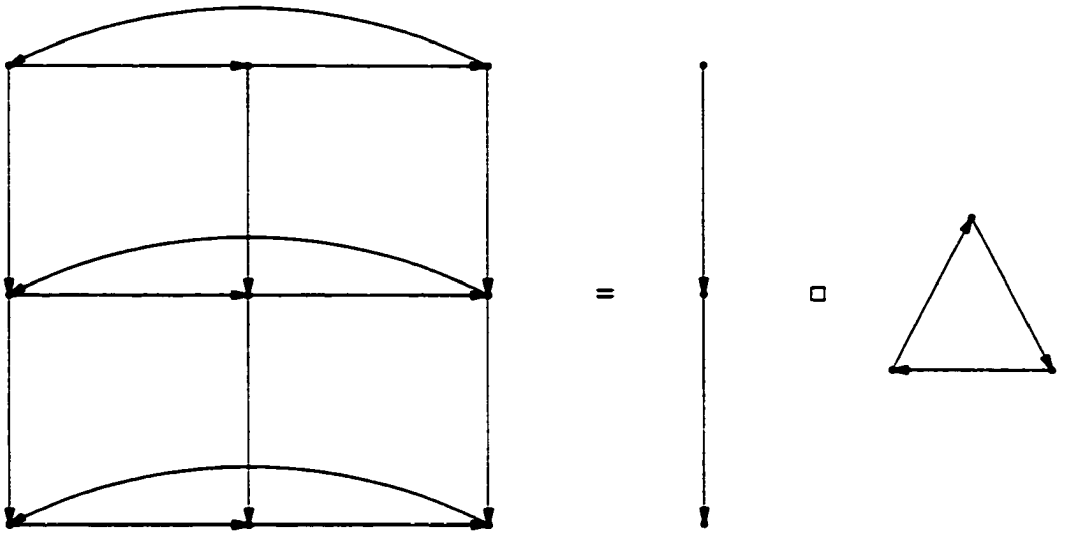

Figure 3.3 The Cartesian factorization of H

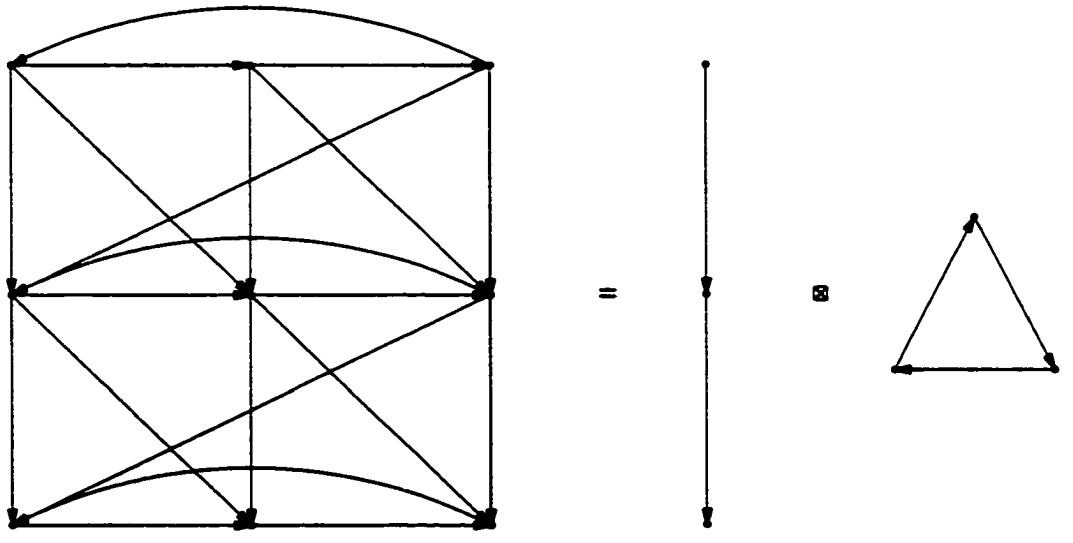

Figure 3.4 The strong factorization of G

CHAPTER 4. THE CONGRUENCE EXTENSION PROPERTY

In this chapter, we consider the complexity of the problem of determining whether a finite algebra $\mathbf{A}$ of finite similarity type has the congruence extension property. Recall that the problem CEP is defined as follows:

$$\text{CEP} = \{\mathbf{A} : \mathbf{A} \text{ has the congruence extension property}\}.$$

Given an algebra $\mathbf{A}$, the problem is to determine whether $\mathbf{A} \in$ CEP. We prove that CEP is complete for polynomial time.

Definition 4.0.1. An algebra $\mathbf{A}$ has the *congruence extension property* if for all $\mathbf{B} \leq \mathbf{A}$ and for all $\theta \in \text{Con}(\mathbf{B})$, there exists a $\overline{\theta} \in \text{Con}(\mathbf{A})$ such that $\overline{\theta} \restriction_B = \theta$, where $\overline{\theta} \restriction_B := \overline{\theta} \cap B^2$.

For groups, there is a one-to-one correspondence between congruences and normal subgroups. Let $\mathbf{G}$ be a group with a normal subgroup $\mathbf{N}$. Then $\theta_N = \{(a,b) \in G^2 : aN = bN\}$ is a congruence on $\mathbf{G}$. Conversely, if θ is a congruence on $\mathbf{G}$, then $\mathbf{N}_\theta = e/\theta = \{g \in G : (g,e) \in \theta\}$ is a normal subgroup of $\mathbf{G}$, where e is the identity of the group. Thus, for groups we can express the congruence extension property in terms of normal subgroups: A group $\mathbf{G}$ has the congruence extension property if for all $\mathbf{H} \leq \mathbf{G}$ and for all $\mathbf{N} \trianglelefteq \mathbf{H}$, there exists an $\overline{\mathbf{N}} \trianglelefteq \mathbf{G}$ such that $\overline{\mathbf{N}} \cap \mathbf{H} = \mathbf{N}$.

For example, suppose $\mathbf{G}$ is an Abelian group, and let $\mathbf{H} \leq \mathbf{G}$. Then since $\mathbf{G}$ is Abelian, $\mathbf{H} \trianglelefteq \mathbf{G}$. Let $\mathbf{N} \trianglelefteq \mathbf{H}$. Then $\mathbf{N} \leq \mathbf{G}$, and since $\mathbf{G}$ is Abelian, $\mathbf{N} \trianglelefteq \mathbf{G}$. Take $\overline{\mathbf{N}} = \mathbf{N}$, and clearly, $\overline{\mathbf{N}} \cap \mathbf{H} = \mathbf{N}$. Therefore, all Abelian groups have the congruence extension property. Also note that an algebra with no proper subalgebras trivially has the congruence extension property.

Perhaps the easiest example of an algebra which does not have the congruence extension property is a simple algebra $\mathbf{A}$ with a nonsimple subalgebra $\mathbf{B}$. As a specific example, the group

$\mathbf{A}_5$ of even permutations on five letters is simple, but the subgroup $\mathbf{B}$ of $\mathbf{A}_5$ with subuniverse $B = \{(12)(34), (13)(25), (14)(35), (15)(24), (23)(45), (14325), (15234), (12453), (13524), (1)\}$ has a normal subgroup $\mathbf{N}$ with $N = \{(14325), (15234), (12453), (13524), (1)\}$. Therefore, $\mathbf{A}_5$ does not have the congruence extension property.

There are known complexity results for many algorithmic problems in algebra. In proving that the problem CEP is complete for polynomial time, we make use of two of these results. Define GEN-SUBALG to be the following problem:

$$\text{GEN-SUBALG} = \{\langle \mathbf{A}, X, a\rangle : X \subseteq A,\ a \in A,\ \text{and } a \in \mathrm{Sg}^{\mathbf{A}}(X)\}.$$

In (12) Jones and Laaser proved that GEN-SUBALG is complete for $\mathbf{P}$.

Define the problem GEN-CON as follows:

$$\text{GEN-CON} = \{\langle \mathbf{A}, \theta, a, b\rangle : a, b \in A,\ \theta \subseteq A^2,\ \text{and } (a,b) \in Cg^{\mathbf{A}}(\theta)\}.$$

In (3) Bergman and Slutzki proved that GEN-CON is compete for nondeterministic log-space. Recall from Chapter 2 that $\mathbf{NL} \subseteq \mathbf{P}$.

Our proof that CEP is in $\mathbf{P}$ uses a corollary to a theorem from Alan Day (6). Before stating the theorem, we need one more definition. An algebra $\mathbf{A}$ has the *principal congruence extension property* if for any subalgebra $\mathbf{B} \leq \mathbf{A}$, every principal congruence on $\mathbf{B}$ is the restriction of some congruence on $\mathbf{A}$. We state Day's Theorem in terms of a single algebra, but note that it holds for an equational class.

Day's Theorem. *For an algebra* $\mathbf{A}$*, the following are equivalent:*

1. $\mathbf{A}$ *satisfies the congruence extension property.*
2. $\mathbf{A}$ *satisfies the principal congruence extension property.*
3. *For all* $\mathbf{B} \leq \mathbf{A}$ *and all* $a, b \in B$, $\mathrm{Cg}^{\mathbf{B}}(a,b) = \mathrm{Cg}^{\mathbf{A}}(a,b) \restriction_B$.

Corollary 4.0.2. $\mathbf{A}$ *satisfies the congruence extension property if and only if for all* $a, b, c, d \in A$, $(c,d) \in \mathrm{Cg}^{\mathbf{A}}(a,b)$ *iff* $(c,d) \in \mathrm{Cg}^{\mathbf{B}}(a,b)$, *where* $\mathbf{B}$ *is the subalgebra of* $\mathbf{A}$ *generated by* $\{a, b, c, d\}$.

Proof. We will show that the third condition of Day's Theorem is equivalent to the condition

$$\forall a, b, c, d \in A,\ (c, d) \in \mathrm{Cg}^{\mathbf{A}}(a, b) \text{ iff } (c, d) \in \mathrm{Cg}^{\mathbf{B}}(a, b). \tag{4.1}$$

Let $a, b, c, d \in A$. Define $\mathbf{B}$ as the subalgebra of $\mathbf{A}$ generated by $\{a, b, c, d\}$. Then since $a, b \in B$ and $\mathbf{B} \leq \mathbf{A}$, by the third condition of Day's Theorem, we have $\mathrm{Cg}^{\mathbf{B}}(a, b) = \mathrm{Cg}^{\mathbf{A}}(a, b) \restriction_B$. So, $(c, d) \in \mathrm{Cg}^{\mathbf{B}}(a, b)$ if and only if $(c, d) \in \mathrm{Cg}^{\mathbf{A}}(a, b) \restriction_B$. Since $c, d \in B$, $(c, d) \in \mathrm{Cg}^{\mathbf{A}}(a, b) \restriction_B$ if and only if $(c, d) \in \mathrm{Cg}^{\mathbf{A}}(a, b)$. Therefore, $(c, d) \in \mathrm{Cg}^{\mathbf{A}}(a, b)$ if and only if $(c, d) \in \mathrm{Cg}^{\mathbf{B}}(a, b)$.

For the other direction, suppose $\mathbf{B} \leq \mathbf{A}$, and let $a, b \in B$. Then we have $\mathrm{Cg}^{\mathbf{B}}(a, b) \subseteq \mathrm{Cg}^{\mathbf{A}}(a, b) \restriction_B$, and we need to show the opposite inclusion. Suppose $(c, d) \in \mathrm{Cg}^{\mathbf{A}}(a, b) \restriction_B$. Then c and d must be elements of B. By (4.1), $(c, d) \in \mathrm{Cg}^{\mathbf{A}}(a, b)$ if and only if $(c, d) \in \mathrm{Cg}^{\mathbf{C}}(a, b)$, where $C = \mathrm{Sg}^{\mathbf{A}}(a, b, c, d)$. Since $a, b, c, d \in B$, we have $\mathrm{Sg}^{\mathbf{B}}(a, b, c, d) = \mathrm{Sg}^{\mathbf{A}}(a, b, c, d) = C$. Again by (4.1), we have $(c, d) \in \mathrm{Cg}^{\mathbf{B}}(a, b)$ if and only if $(c, d) \in \mathrm{Cg}^{\mathbf{C}}(a, b)$. Also, $(c, d) \in \mathrm{Cg}^{\mathbf{A}}(a, b)$ if and only if $(c, d) \in \mathrm{Cg}^{\mathbf{A}}(a, b) \restriction_B$ because c and d are elements of B. Thus, $(c, d) \in \mathrm{Cg}^{\mathbf{B}}(a, b)$, so $\mathrm{Cg}^{\mathbf{A}}(a, b) \restriction_B \subseteq \mathrm{Cg}^{\mathbf{A}}(a, b)$. □

Theorem 4.0.3. CEP $\in$ **P**.

Proof. From Corollary 4.0.2 we have the following equivalence:

$$\mathbf{A} \text{ has CEP iff for all } a, b, c, d \in A,\ (c, d) \in \mathrm{Cg}^{\mathbf{B}}(a, b) \Leftrightarrow (c, d) \in \mathrm{Cg}^{\mathbf{A}}(a, b),$$

where $B = \mathrm{Sg}^{\mathbf{A}}\{a, b, c, d\}$. We present an algorithm to check this condition. Assume that $\mathbf{A} = \langle A, F \rangle$, with $A = \{a_1, \ldots, a_n\}$.

Algorithm 2. CEP(**A**)

$n \leftarrow |A|, B \leftarrow \emptyset$

for all $(a_i, a_j, a_k, a_l) \in A^4$ do

for $m = 1$ to n do

If $\langle \mathbf{A}, (a_i, a_j, a_k, a_l), a_m \rangle \in$ GEN-SUBALG, then $B \leftarrow B \cup \{a_m\}$.

od

$\mathbf{B} \leftarrow \langle B, F \restriction_B \rangle$

If $\langle \mathbf{A}, (a_i, a_j), a_k, a_l \rangle \in$ GEN-CON $\oplus$ $\langle \mathbf{B}, (a_i, a_j), a_k, a_l \rangle \in$ GEN-CON $= 1$, then reject.

od

Accept

The symbol $\oplus$ represents the exclusive or operation, so $x \oplus y = 1$ if the the truth value of x is not equal to the truth value of y . For all such quadruples $\{a, b, c, d\} \subseteq A$, B is generated in polynomial time by checking whether $\langle \mathbf{A}, \{a, b, c, d\}, x\rangle \in$ GEN-SUBALG for all elements $x \in A$. The $\Leftrightarrow$ equivalence is checked in nondeterministic log-space using GEN-CON with $\theta = \{(a, b)\}$. □

Theorem 4.0.4. CEP *is complete for* **P**.

Proof. To show that CEP is **P**-hard, we shall give a log-space reduction of GEN-SUBALG to CEP.

Let $\langle \mathbf{A}, X, a\rangle$ be an instance of GEN-SUBALG, where $\mathbf{A} = \langle A, F\rangle$. If $X = \emptyset$ and $\mathbf{A}$ has no nullary operations, then let $\mathbf{A}' = \mathbf{A}_5$. Otherwise, construct $\mathbf{A}'$ in the following manner.

Assuming that $A \cap \{0, 1\} = \emptyset$, let $A' = A \cup \{0, 1\}$ be the universe of $\mathbf{A}'$. Note that if $A \cap \{0, 1\} \neq \emptyset$, then we can replace 0 and 1 with two symbols which are not in A. For all $b \in A \cup \{1\}$, define an operation g_b as follows:

$$g_b(x) = \begin{cases} b & \text{if } x = a \\ x & \text{otherwise.} \end{cases}$$

If $X \neq \emptyset$, then there exists $c_1 \in X$. On the other hand, if $X = \emptyset$, then $\mathbf{A}$ has a nullary operation, say c_1. In both cases, define

$$h(x, y) = \begin{cases} c_1 & \text{if } x = 1 \text{ and } y = a \\ 0 & \text{otherwise.} \end{cases}$$

Now let $\mathbf{A}' = \langle A \cup \{0, 1\}, F \cup \{g_b : b \in A \cup \{1\}\} \cup \{h\} \cup \{c_i : c_i \in X\}\rangle$, where the c_i's are constant operations and for all $f \in F$, $f(x_1, \ldots, x_k) = 0$ if $\{x_1, \ldots, x_k\} \cap \{0, 1\} \neq \emptyset$.

For completeness, we need to check that $\langle \mathbf{A}, X, a\rangle \in$ GEN-SUBALG $\Leftrightarrow \mathbf{A}' \in$ CEP. Consider first the case where $X = \emptyset$ and $\mathbf{A}$ has no nullary operations. Then clearly $a \notin \mathrm{Sg}^{\mathbf{A}}(X) = \emptyset$. Since $\mathbf{A}' = \mathbf{A}_5$, $\mathbf{A}' \notin$ CEP, and the above equivalence holds.

For the remaining cases, we first show that $\langle \mathbf{A}, X, a\rangle \in$ GEN-SUBALG $\Rightarrow \mathbf{A}' \in$ CEP. Suppose $\langle \mathbf{A}, X, a\rangle \in$ GEN-SUBALG, i.e., $a \in \mathrm{Sg}^{\mathbf{A}}(X)$. Let $\mathbf{C} = \langle A, F \cup \{g_b : b \in A\}\rangle$. If $a \in \mathrm{Sg}^{\mathbf{A}}(X)$ then $a \in \mathrm{Sg}^{\mathbf{C}}(X)$, since $\mathbf{C}$ is an expansion of $\mathbf{A}$. For every element $b \in A$, $b = g_b(a) \in \mathrm{Sg}^{\mathbf{C}}(a)$, and since $a \in \mathrm{Sg}^{\mathbf{C}}(X)$, we have $\mathrm{Sg}^{\mathbf{C}}(a) \subseteq \mathrm{Sg}^{\mathbf{C}}(X)$. So, $A \subseteq \mathrm{Sg}^{\mathbf{C}}(X)$. We also have $\mathrm{Sg}^{\mathbf{C}}(X) \subseteq A$, since A is the universe of $\mathbf{C}$. Thus, $\mathrm{Sg}^{\mathbf{C}}(X) = A$.

For all $c_i \in X$, c_i is a constant symbol of $\mathbf{A}'$ and $\mathrm{Sg}^{\mathbf{C}}(X) = A$, so every subuniverse of $\mathbf{A}'$ must contain A. Since $a \in A$ and g_1 is a basic operation of $\mathbf{A}'$, any subuniverse of $\mathbf{A}'$ must contain $g_1(a) = 1$. Then $h(1,1) = 0$ must also be contained in any subuniverse of $\mathbf{A}'$. Therefore, $A' = A \cup \{0,1\}$ is the only subuniverse of $\mathbf{A}'$. In other words, $\mathbf{A}'$ has no proper subalgebras.

It follows that $\mathbf{A}' \in$ CEP, so we have shown that $\langle \mathbf{A}, X, a\rangle \in$ GEN-SUBALG $\Rightarrow \mathbf{A}' \in$ CEP. Now suppose $a \notin \mathrm{Sg}^{\mathbf{A}}(X)$. We need to show that $\mathbf{A}' \notin$ CEP.

Let $B = \mathrm{Sg}^{\mathbf{A}}(X) = \{b_1, b_2, \ldots, b_m\}$, and let $\mathbf{B}'$ be the subalgebra of $\mathbf{A}'$ with subuniverse $B' = B \cup \{0,1\}$. It is straightforward to check that B' is a subuniverse of $\mathbf{A}'$. Let $\theta = \{(0,0),(0,1),(1,0),(1,1)\} \cup 1_B$ so that θ is the equivalence relation on B' with partition $\{\{0,1\},\{b_1,\ldots b_m\}\}$.

To prove $\theta \in \mathrm{Con}(\mathbf{B}')$, we need to show that the basic operations of $\mathbf{B}'$ preserve θ. Since a is not an element of B', for every $b \in B \cup \{1\}$, g_b acts as the identity map on B', and for all pairs x, y in B', $h(x,y) = 0$. So, $\{g_b : b \in B \cup \{1\}\}$ and h preserve θ. Clearly, the constant operations also preserve θ.

Since B is a subuniverse of $\mathbf{A}$, B is closed under all operations f in F. To show that F preserves θ, first consider all pairs $b_i, b_j \in B$. By the definition of θ, $(b_i, b_j) \in \theta$ for all $1 \leq i, j \leq m$. For x_i, y_i in B, $i = 1, \ldots, k$, $(f(x_1,\ldots,x_k), f(y_1,\ldots,y_k)) = (b_i, b_j)$ for some $b_i, b_j \in B$. If x_i and y_i are in $\{0,1\}$ for some $1 \leq i \leq k$, then $(f(x_1,\ldots,x_k), f(y_1,\ldots,y_k)) = (0,0)$. Thus, F preserves θ, and θ is in $\mathrm{Con}(\mathbf{B}')$.

It remains to be shown that θ does not have an extension in $\mathrm{Con}(\mathbf{A}')$. Let $\alpha \in \mathrm{Con}(\mathbf{A}')$. If $(0,1) \notin \alpha$, then $\alpha \restriction_{B'} \neq \theta$ since $(0,1) \in \theta$. On the other hand, if $(0,1) \in \alpha$, then $(h(0,a), h(1,a)) = (0, c_1) \in \alpha$. But then $\alpha \restriction_{B'} \neq \theta$, since 0 and c_1 are elements of B' but

$(0, c_1)$ is not in θ.

We construct the output algebra $\mathbf{A}'$ as the group $\mathbf{A_5}$ or by adding operations to the input algebra $\mathbf{A}$. The operations are stored as tables, and each row of an operation table can be determined by one pass through the input. The space used in constructing the tables can also be reused, so the reduction can be computed in log-space. Therefore, CEP is **P**-complete. □

CHAPTER 5. OPEN PROBLEMS

There are many open problems in computational complexity, both in graph theory and universal algebra. We discuss a few that are related to results in this paper. In fact, exploring one of these open problems in algebra led to the digraph decomposition result presented in this paper. Specifically, that problem is determining whether an algebra is directly indecomposable, where an algebra is defined to be *directly indecomposable* if it is not isomorphic to a direct product of two nontrivial algebras. We formally define the problem DI as follows:

$$\mathrm{DI} = \{\mathbf{A} : \mathbf{A} \text{ is directly indecomposable}\}.$$

There are often connections between problems in graph theory and problems in algebra. Clearly, the problem DI has some connections to the graph factorization problems, but a few complications arise. For instance, with algebras, there is only one standard product, but with graphs, there are several. The weak product seems to be the most connected to the direct product of algebras, and it also appears to be the most complicated of the graph products, as far as the factoring problem is concerned.

Both the Cartesian and the strong product results about graph factorizations have been extended to digraphs. However, the problem of decomposing digraphs with respect to the weak direct product is still open. According to Imrich (10), if all factors are connected, there is no obvious reason why the complexity of factoring digraphs under the weak product should be higher than the complexity of factoring undirected graphs with respect to the weak product. So, it appears there should be a polynomial-time algorithm to decompose digraphs with respect to the weak product. However, at this point, we have been unable to design such an algortihm.

For disconnected graphs or digraphs, the problem of finding the Cartesian decomposition is at least as hard as the graph isomorphism problem (8), which is known to be in **NP** (17). Since

the algorithms for factoring (di)graphs with respect to the strong and weak direct products utilize the Cartesian factoring algorithms, the complexity of factoring disconnected (di)graphs under either of these product also appears to be at least as hard as graph isomorphism. This suggests that the problem DI could be as hard as algebra isomorphism, which has the same complexity as graph isomorphism. In addition, for the weak direct product, there are no results regarding the factorization of bipartite graphs or digraphs.

Even though there are polynomial time algorithms for many of these decomposition problems, perhaps faster algorithms could be designed. Indeed, this is already the case for the Cartesian product of undirected graphs, in which the first algorithm presented has complexity $O(n^{4.5})$, and the most recent algorithm has complexity $O(m \log n)$, where m is the number of edges and n is the number of vertices of the graph. Also, there are no completeness results, so it could be possible for these problems to be in a lower complexity class such as **NL**.

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